

**GUIDANCE DOCUMENTS ON MEASUREMENTS & MODELLING  
OF NOVEL AIR QUALITY POLLUTANTS:**

**DETERMINISTIC URBAN MODELLING: PM & PN**



**RI-URBANS**

**Research Infrastructures Services Reinforcing Air Quality  
Monitoring Capacities in European Urban & Industrial Areas  
(GA n. 101036245)**

**by**



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**ABBREVIATIONS**

<b>ACTRIS</b>	Aerosols, Clouds and Trace gases Research InfraStructure
<b>ADMS-Urban</b>	Local scale dispersion model with gaussian-based approach
<b>BC</b>	Black carbon
<b>CAMS</b>	Copernicus Atmosphere Monitoring Service
<b>CHIMERE</b>	Chemical transport model with eulerian approach
<b>CityChem</b>	Model for the chemical transformation of pollutants
<b>CTM</b>	Chemistry transport model
<b>eBC</b>	Equivalent black carbon
<b>EC</b>	Elemental carbon
<b>EMEP</b>	European Monitoring and Evaluation Programme
<b>EPISODE</b>	Eulerian model with a sub-grid Gaussian dispersion for street canyons
<b>Fac2</b>	Fraction 2, meaning fraction of data within a factor of 2 of observations
<b>MFB</b>	Mean Fractional Bias
<b>MFE</b>	Mean Fractional Error
<b>MUNICH</b>	Model of Urban Network of Intersecting Canyons and Highways
<b>PM</b>	Particulate matter
<b>PM<sub>0.01</sub></b>	Mass concentration of particles <0.01 µm
<b>PM<sub>0.1</sub></b>	Mass concentration of particles <0.1 µm
<b>PM<sub>1</sub></b>	Mass concentration of particles <1 µm
<b>PM<sub>2.5</sub></b>	Mass concentration of particles <2.5 µm
<b>PM<sub>10</sub></b>	Mass concentration of particles <10 µm
<b>PN</b>	Particle number
<b>PNC</b>	Particle number concentration
<b>RI-URBANS</b>	Research Infrastructures Services Reinforcing Air Quality Monitoring Capacities in European Urban & Industrial AreaS EU-project
<b>SSH</b>	Aerosol model for physical-chemical transformation undergone by aerosols in the troposphere
<b>UFP</b>	Ultrafine particle(s)
<b>WRF</b>	Weather Research & Forecasting Model

**CHEMICAL SPECIES**

<b>CO</b>	Carbon monoxide
<b>NO<sub>2</sub></b>	Nitrogen dioxide
<b>O<sub>3</sub></b>	Ozone



## 1. ABOUT THIS DOCUMENT

This document was prepared as part of the "Research Infrastructures Services Reinforcing Air Quality Monitoring Capacities in European Urban & Industrial AreaS" (RI-URBANS) EU-project that connects the atmospheric observation expertise from Aerosols, Clouds and Trace gases Research InfraStructure (ACTRIS) as well as the urban air quality observation capacities of the regulatory air quality monitoring networks.

This document is a guide for the service tool for deterministic modelling atmospheric particle mass (PM) and number (PN) concentrations at urban scale.

Pollutants such as nitrogen dioxide (NO<sub>2</sub>), PM<sub>2.5</sub>, black carbon (BC) and particle number (PN) may strongly impact the health of population. Furthermore, their concentrations are often observed to be particularly high over cities, with strong urban heterogeneities. In cities, concentration of NO<sub>2</sub>, BC and PN and to a lesser extent PM<sub>2.5</sub> are particularly high along traffic axes and in streets. To estimate the outdoor concentration exposure of population, maps are required at spatial scales below 100 m, at the minimum, to be able to differentiate the street from the urban background concentrations. Hourly time resolution is desirable.

At the European and regional scales, chemistry-transport models (CTM) are commonly used to map NO<sub>2</sub>, CO, O<sub>3</sub> and PM<sub>2.5</sub>, PM<sub>10</sub> (e.g. Copernicus Atmosphere Monitoring Service CAMS). Over cities, chemistry-transport models may also be used using a nested domain approach to map urban background concentrations. The horizontal resolutions are typically coarser than 1x1 km<sup>2</sup>. However, they cannot capture the city heterogeneities, which may be more or less significant depending on the pollutant. They are found to be more important for NO<sub>2</sub>, BC and PN than for PM<sub>2.5</sub> (Park et al. 2024).

Local-scale modelling over cities is particularly suitable for representing the concentrations of pollutants that are highly influenced by urban heterogeneity. Multi-scale deterministic models, which combine a regional-scale CTM and a local-scale model may also be used to represent the local variations while taking urban and regional transport into account.

In this service tool, three models based on different methodologies and complexity are presented.

- The multi-scale Eulerian model CHIMERE/MUNICH/SSH-aerosol (3-dimensional (3-D) Eulerian CTM grid model with sub-grid Eulerian dispersion and chemistry/aerosol dynamic at all scales).
- The multi-scale hybrid model Episode-CityChem (3-D Eulerian CTM grid model with sub-grid Gaussian dispersion).
- The Gaussian-based model ADMS-Urban.

In addition to the above-mentioned deterministic approaches, statistical mapping methodologies are also used to produce very high-resolution map of air pollutant concentrations. Various level of complexity of statistical, geostatistical, or machine learning regression methodologies can be used in that context. At present, the majority of such products are targeted at annual mean concentration of past historical periods. And such information is particularly useful to inform epidemiological studies and health impact assessment. But for short term forecasts or future scenarios to guide the effectiveness of policy making, deterministic models remain an essential tool, even if those are more and more coupled with machine learning pre and post processing algorithm.

**This is a RI-URBANS/ACTRIS guidance for this specific service tool that is part of the RI-URBANS deliverable D46 (D6.1, containing guidance for all service tools provided in the project) with the support for publication from AXA Research Fund to build up the final dissemination D55 (D7.6). Any dissemination of results must indicate that it**

reflects only the author's view and that the European Commission is not responsible for any use that may be made of the information it contains.

## 2. INPUT DATA

For the regional-scale modelling, chemistry-transport models require several input data that are specific to the domain of study: meteorology, boundary conditions, emission inventory. Meteorological fields may be obtained by different agencies, such as ECMWF (European Centre for Medium-Range Weather Forecasts), NCEP (National Centers for Environmental Prediction), and downscaling down to the urban scale may be performed using different models, such as WRF (Weather Research & Forecasting Model). Boundary conditions may be obtained from global models or regional reanalysis, such as those provided by CAMS, and/or from a nested domain approach down to the city scale. Emission inventories using top-down approach are available at the European scale (e.g. EMEP, CAMS), and they may be downscaled to the city scale. Tools for this purpose may be embedded in chemistry-transport models (e.g. CHIMERE, Menut et al. 2021). In the frame of RI-URBANS, a spatial disaggregation method of CAMS-REG emissions is implemented, based on developments of the UrbEm tool (Ramacher et al. 2021), which produces high resolution -per 1x1 km<sup>2</sup> area- emission data (consistent to the CAMS-REG structure and contents), with the flexibility for point and/or line data, to use for local-scale modelling. This is detailed in the Service Tool 'EMISSION INVENTORIES FOR REGIONAL AND URBAN SCALE MODELLING APPLICATIONS'. Bottom-up inventories may also be used.

For local-scale modelling, hourly road-network emissions are also needed. Correction of the traffic flow and hence of the traffic emissions using traffic count loops may improve the modelling for some pollutants, such as BC and PN concentrations (Park et al 2024). Not only emissions, but also the characteristics of the main streets (lengths, widths and heights) are necessary for local-scale simulations.

## 3. MODEL EVALUATION

Evaluation of the validity of maps of modelled air pollutant concentrations across cities is challenging because of the generally spatially sparse monitoring data. As large gradients are observed for some pollutants, such as NO<sub>2</sub>, BC and PNC, but also to a lower extent for PM<sub>2.5</sub>, it is necessary to evaluate the models at different types of stations characteristic of urban areas (traffic, urban background, suburban).

In this service tool, the simulated concentrations are evaluated by comparison to measurement stations using statistics such as Mean Fractional Bias (MFB), Mean Fractional Error (MFE), and the fraction 2 (Fac2). Two model performance criteria are determined. The less strict one is met if both MFE < 75% and MFB < ±50%, and the strictest model performance goal is met if MFE < 50% and MFB < ±30% (Boylan and Russell, 2006). The Fac2 statistic is also evaluated. It is the fraction of modelled data within a factor of 2 of observations. It should be higher than 0.5 for the strictest criteria and 0.3 for a less strict criteria (Hanna and Chang 2012).

For comparisons to observations, as the model simulates the mass of EC, the eBC observed concentrations are corrected using a harmonization factor, following Savadkoobi et al. (2024). For PNC, particles of diameters larger than 10 nm are considered here.

## 4. ADDED VALUE OF THE MODELLING

For pollutants with large urban concentration gradients, modelling allows to map the concentrations down to the street scale over the whole city, with a detailed temporal resolution (hourly). Because the models rely on an



emission inventory and a detailed representation of the physical processes occurring in the atmosphere, an accurate representation of the concentrations at several types of station and for several time periods and seasons give us confidence in the model ability to map accurately the pollutant concentrations.

## 5. INFORMATION ON MODELLING METHODS AND QUALITY CONTROL

Three approaches based on different methodologies are proposed:

- A Eulerian approach with a chemistry-transport model (CHIMERE (Menut et al. 2021) or Polair3D (Sartelet et al. 2022)) coupled to the street-network model MUNICH, with coherent gaseous chemistry and aerosol dynamics at all scales. Examples of this multi-scale Eulerian approach are available in Lugon et al. (2022), Sarica et al. (2023), Maison et al. (2024), Squarcioni et al. (2024), Park et al. (2024). All the pollutants modelled at the regional-scale with the chemistry-transport model are also modelled down to the street scale, as the same chemistry and aerosol dynamics model is used (SSH-aerosol, Sartelet et al. 2020). The model chain has been extensively evaluated for NO<sub>2</sub> and PM<sub>2.5</sub> concentrations, and an example over Paris including modelling of PN and BC is detailed below and in Park et al. (2024). Modelling of secondary organic aerosols down to the street scale may also be performed as shown in Sartelet et al. (2024).
- A hybrid approach, i.e. the chemistry-transport model (CTM) which combines a Eulerian model with a sub-grid Gaussian dispersion for street canyons (EPISODE) and with an extension treating the chemical transformation of pollutants (CityChem) (Karl et al., 2019; Lasne et al., 2023). In this chain, NO<sub>2</sub> and PM<sub>2.5</sub> may be modelled down to a 100 m x 100 m scale, and an example over Athens is detailed below.
- A Gaussian-based approach with the model ADMS-Urban, which can represent NO<sub>2</sub> and PM<sub>2.5</sub> concentrations down to 10 m x 10 m scale, and has been extended to model PNC. An example over Birmingham is detailed below and in Zhang et al. (2023).

To illustrate the model capabilities, set-up and results, simulations are performed for each model for a winter and a summer period.

### 5.1 Eulerian approach with the CHIMERE/MUNICH/SSH-aerosol chain

In the example over Paris, the segments of the street network are those defined by Airparif, the Île-de-France air quality agency. They correspond to the main roads. The main street characteristics are obtained from the French BDTOPO database (<https://geoservices.ign.fr/bdtopo>). The street network is made of 4655 streets and extends over the city of Paris and its nearby suburbs.

Regional-scale concentrations are simulated with the CHIMERE model (Menut et al. 2021) coupled to the street network MUNICH. The concentrations of NO<sub>2</sub>, PM<sub>2.5</sub>, PNC, eBC and other particle compounds (e.g. organic aerosols) are simulated. All the gas and particle compounds simulated at the regional scale are also simulated down to the street scale. Indeed, the chain CHIMERE/MUNICH use the same aerosol module (SSH-aerosol, Sartelet et al. 2020) at both the regional and local scales, allowing to consider the dynamic of particles at all scales. In the CHIMERE/MUNICH chain, nested domains are considered using CAMS boundary conditions over Europe. The smallest domain of CHIMERE simulation is discretized with a 1 km x 1 km resolution over Greater Paris. A zoom is performed in the streets of Paris, which are explicitly represented using a Eulerian approach with the street network MUNICH. Using a Eulerian approach at the street scale leads to a direct exchange between the background and the street, making it possible to accurately estimate the formation of secondary pollutants, and avoiding potential double counting of traffic emissions when calculating the background and the street concentrations.

To illustrate the impact of bottom-up versus top-down emission inventories, two different emission inventories are used: the EMEP top-down emission inventory, and the bottom-up Airparif inventory. In the Airparif inventory, the traffic fleet and emissions are specific of the period of simulation (winter 2020 and summer 2022 here). The road traffic emissions data were produced based on the results obtained using the Heaven system originally developed in 2001 as part of the European project of the same name in partnership with the road traffic management departments of the City of Paris and the Direction Régionale de l'Équipement d'Île-de-France. Since then, this

system has been regularly updated on all its components: emission factors, vehicle fleets, traffic model, real-time countings, network, etc., in order to have the most recent information on vehicle emissions in the Paris region. The strength of this system is to use a traffic model that is corrected from the count data received in near real time. In the chain CHIMERE/MUNICH, the regional-scale traffic emissions were estimated by aggregating the local-scale emissions.

Number emissions and the size distribution at emissions were estimated from the emission inventory using the methodology detailed in Sartelet et al. (2022) and Park et al. (2024). The emission inventories provide estimations of PM<sub>2.5</sub> emissions for the different activity sectors. To distribute PM<sub>2.5</sub> emissions in the modelled particle size sections, first emissions of particles in the range PM<sub>0.1</sub>-PM<sub>1</sub> and PM<sub>0.01</sub>-PM<sub>0.1</sub> are estimated using the PM<sub>1</sub>/PM<sub>2.5</sub> and PM<sub>0.1</sub>/PM<sub>1</sub> ratios given in Sartelet et al. (2022) for each activity sector. The emissions in each of the size ranges: PM<sub>0.01</sub>-PM<sub>0.1</sub>, PM<sub>0.1</sub>-PM<sub>1</sub>, and PM<sub>1</sub>-PM<sub>2.5</sub> are distributed amongst the model size sections with an algorithm that conserves mass and number. Note that for the residential sector, the lowest diameter considers for emission is 80 nm (against 10 nm for the other sectors).

For comparisons to observations, the eBC observed concentrations are normalized using a harmonization factor, following Savadkoobi et al. (2024). A harmonization factor of 1.79 and 1.70 was determined for Paris in the summer 2022 and the winter 2020/2021 respectively using EC and eBC collocated measurements at Châtelet-les-Halles station, which is a urban background station operated by Airparif in the centre of Paris.

The simulation was performed with the set-up detailed in Park et al. (2024) between 2 June 2022 and 31 July 2022 for the Summer period, and between 7 December 2020 and 28 February 2021 for the Winter period. The model comparisons to observations is show in Tables 1 to 4 for NO<sub>2</sub>, eBC, PM<sub>2.5</sub> and PN respectively. The modelled concentrations satisfy the strictest performance criteria for all pollutants. At background stations, the statistics are similar if EMEP or Airparif inventory is used for PM<sub>2.5</sub>, but the bottom-up Airparif inventory with detailed traffic emission leads to better statistics for NO<sub>2</sub>, eBC and PN than the top-down inventory EMEP. This is more marked in summer than in winter.

For PNC, due to the lack of PN measurement at traffic stations, the concentrations simulated in summer 2022 are compared with the concentrations observed in summer 2021 at two traffic sites in Paris (BP\_EST and HAUSS), as documented in the Airparif report (Airparif, 2021). The average PN concentrations measured in the summer 2021 were 17,000 # cm<sup>-3</sup> and 21 300 # cm<sup>-3</sup> respectively for particles of diameters between 10 and 400 nm. The simulated PN concentrations are 14,500 # cm<sup>-3</sup> at HAUSS and 30,700 # cm<sup>-3</sup> at BP\_EST, suggesting a bias of 15% at HAUSS and 40% at BP\_EST. The wider bias at BP\_EST is certainly due to the 10 nm cut-off diameter for the particles. At HAUSS, most of the particle number concentrations is between 10 nm and 400 nm, while many particles are observed between 5 and 10 nm at BP\_EST because of the higher importance of vehicle emissions. Note that a proportion of primary particles with diameters smaller than 10 nm may be represented in the modelling approach proposed here. Although there is a difference in the periods of measurement and simulation, the simulated PN concentrations are roughly consistent with the measured ones, and the concentrations in the streets and at the traffic sites are much higher than those in the urban background.

**Table 1.** NO<sub>2</sub> model to measurement comparisons at background and traffic stations for Summer and Winter.

NO <sub>2</sub>	Station	N of Stations	Obs (µg m <sup>-3</sup> )	Emissions	Sim (µg m <sup>-3</sup> )	MFE (%)	MFB (%)	FAC2 (%)
Summer	Background	21	15.0	Airparif	14.7	32	0	90
				EMEP	17.5	35	18	87
	Traffic	10	40.0	Airparif	38.3	31	0	92
Winter	Background	21	24.7	Airparif	25.0	30	2	93
				EMEP	26.1	42	-4	80
	Traffic	9	43.4	Airparif	52.1	28	19	96

**Table 2.** eBC model to measurement comparisons at background and traffic stations for Summer and Winter.

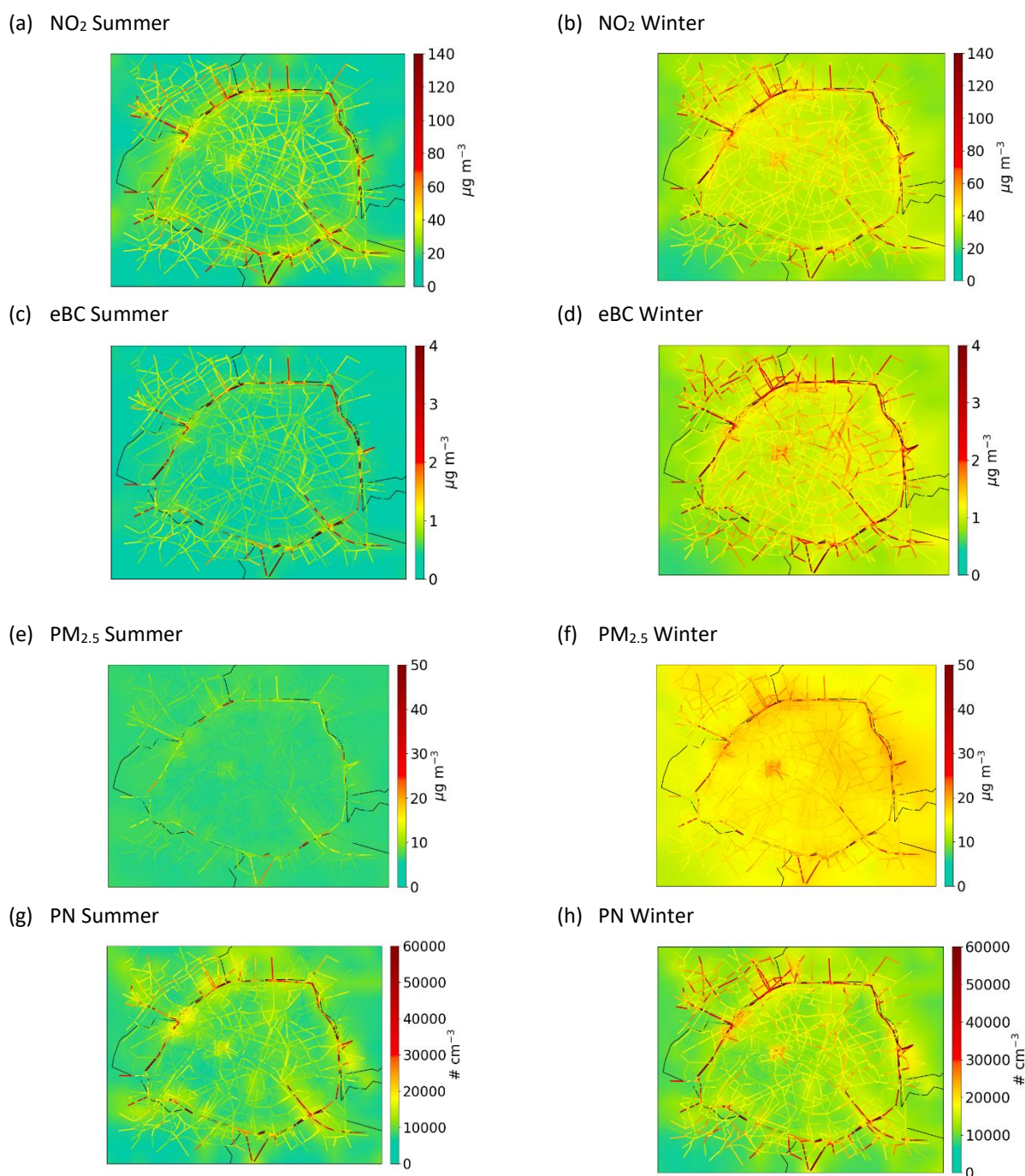
eBC	Station	N of Stations	Obs ( $\mu\text{g m}^{-3}$ )	Emissions	Sim. ( $\mu\text{g m}^{-3}$ )	MFE (%)	MFB (%)	FAC2 (%)
Summer	Background	4	0.36	Airparif	0.44	39	-8	80
				EMEP	0.54	43	30	79
	Traffic	3	1.26	Airparif	1.26	38	15	89
Winter	Urban	5	0.69	Airparif	0.79	43	22	79
				EMEP	0.85	49	26	69
	Traffic	2	1.9	Airparif	2.2	46	28	79

**Table 3.** PM<sub>2.5</sub> model to measurement comparisons at background and traffic stations for Summer and Winter.

PM <sub>2.5</sub>	Station	N of Stations	Obs ( $\mu\text{g m}^{-3}$ )	Emissions	Sim ( $\mu\text{g m}^{-3}$ )	MFE (%)	MFB (%)	FAC2 (%)
Summer	Background	4	7.2	Airparif	6.8	30	0	92
				EMEP	7.3	30	8	91
	Traffic	3	11.2	Airparif	9.9	27	-10	95
Winter	Background	5	12.2	Airparif	13.2	39	17	84
				EMEP	14.2	41	24	81
	Traffic	1	17.2	Airparif	22.0	31	23	93

**Table 4.** PN model to measurement comparisons at background and traffic stations for Summer and Winter.

PNC	Station type	N of Stations	Obs ( $\mu\text{g m}^{-3}$ )	Emissions	Sim ( $\mu\text{g m}^{-3}$ )	MFE (%)	MFB (%)	FAC2 (%)
Summer	Background	4	8176	Airparif	8173	25	4	98
				EMEP	10611	35	27	89
Winter	Background	5	7091	Airparif	8025	43	22	79
				EMEP	10112	48	32	81



**Figure 1.** NO<sub>2</sub> [(a) and (b)], BC [(c) and (d)], PM<sub>2.5</sub> [(e) and (f)], and PNC [(g) and (g)] concentrations simulated for summer (left panels) and winter (right panels) using CHIMERE/MUNICH.

## 5.2 Hybrid approach with the EPISODE-CityChem model

The concentration variability and outdoor population exposure to air pollution in Athens was assessed using the multi-scale numerical atmospheric model system CAMS/WRF/EPISODE-CityChem. The core of the system is the chemistry transport model EPISODE-CityChem (Karl et al., 2019). Its comprehensive chemistry scheme is designed for treating complex atmospheric chemistry in urban areas and improved representation of the near-field dispersion. The model performs a specialized treatment on road and over the adjacent urban areas. Specifically, it is fed with hourly road network emissions in a linear format, applies a Gaussian dispersion scheme in the street

canyons, and an extra photochemical scheme over the greater area of road surfaces, gridded in 100x100 m<sup>2</sup> cells. These two schemes are superimposed to the Eulerian treatment of atmospheric processes in the whole 3D urban domain, with a horizontal spatial resolution of 1 km and a 24-layered atmosphere up to 3.7 km.

Local-scale atmospheric simulations are performed for 2019, which is a recent year, free of Covid-related activity restrictions, and with a wind field representative of 2016-2020. Numerical predictions have been evaluated against local air quality measurements from the National regulatory network and from the Panacea RI.

The months used to represent summer are June, July, August and they are December, January, February for winter. Figure 2 shows the NO<sub>2</sub> and PM<sub>2.5</sub> high resolution (100m) concentrations for a mean day in summer and winter as predicted by EPISODE-CityChem. The concentrations of NO<sub>2</sub> tend to be higher along streets with high traffic in both seasons (Figures 2a and b). The spatial distribution of both pollutants is similar with higher NO<sub>2</sub> than PM<sub>2.5</sub> values at the inner-city centre (Figure 2a to d). The concentrations are higher in winter than in summer, especially for PM<sub>2.5</sub> (and for background NO<sub>2</sub>). The contributions of residential emissions from heating tend to increase particle concentrations during wintertime. NO<sub>2</sub> photochemistry is enhanced in Athens during summer-time, which is partly the reason for higher NO<sub>2</sub> concentrations at the traffic sites. Other reasons for seasonal differences include the lower boundary layer during wintertime and the stronger dispersion phenomena during summertime (incl. Etesian winds), which affect concentrations, mainly downwind the road network.

The simulated concentrations (in 100m cells) are evaluated by comparison to measurement stations in Tables 5 and 6. For the 2 pollutants and station types, the mean concentrations compare well to the observations satisfying the model performance criteria (MFE < 75%, MFB < ±50%) and the model performance goal (MFE < 50% and MFB < ±30%) of Boylan and Russell (2006) in most cases.

**Table 5.** NO<sub>2</sub> model to measurement comparisons at (urban) background and (traffic) roadside stations in Athens for summer and winter.

NO <sub>2</sub>	Station type	N of stations	Obs (µg m <sup>-3</sup> )	Sim (µg m <sup>-3</sup> )	MFE (%)	MFB (%)	FAC2 (%)
Summer	Background	4	19.5	13.5	22	-9	40
	Traffic	4	59.6	44.0	24	-9	50
Winter	Background	4	26.0	14.3	95	-72	35
	Traffic	4	51.6	41.4	41	-11	59

**Table 6.** As in Table 5 but for PM<sub>2.5</sub>

PM <sub>2.5</sub>	station type	No of stations	Obs (µg m <sup>-3</sup> )	Sim (µg m <sup>-3</sup> )	MFE (%)	MFB (%)	FAC2 (%)
Summer	Background	1	12.6	15.3	30	20	96
	Traffic	2	15.0	15.1	9	0	94
winter	Traffic	2	23.1	17.6	67	-30	72



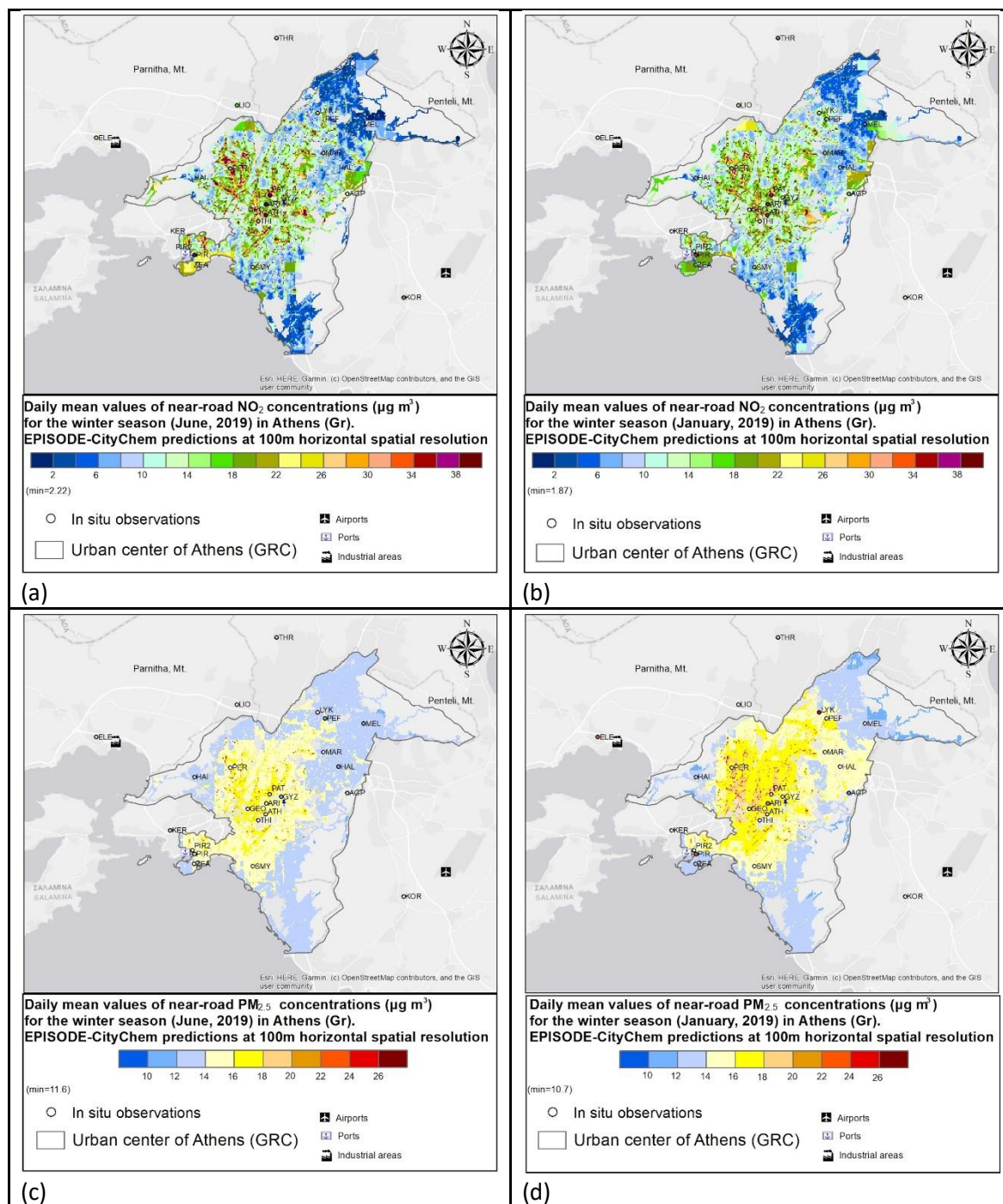


Figure 2. NO<sub>2</sub> [(a) and (b)], PM<sub>2.5</sub> [(c) and (d)], near-road concentrations (µg m<sup>-3</sup>) over Athens simulated for summer (left panels) and winter (right panels) using EPISODE-CityChem.

### 5.3 Gaussian-based approach with the ADMS-Urban model

The local scale ADMS-Urban dispersion model has been used for the Birmingham Pilot to generate high resolution air quality datasets for NO<sub>2</sub>, PM<sub>2.5</sub> and UFPs (Zhong et al., 2021; Zhong et al., 2023). The ADMS-Urban is a quasi-Gaussian plume air dispersion model that represents the structure of the atmospheric boundary layer using meteorological parameters. Birmingham Airport site is an appropriate synoptic meteorological measurement site, which was used to drive the atmospheric dispersion in the model. Background concentration files were created using observation data from a variety of rural background sites (available via the UK Automatic Urban and Rural

Network, AURN) surrounding the West Midlands modelling area. The upwind background site for each hour over the year was selected based on the monitored wind direction at that hour for NO<sub>2</sub>, and PM<sub>2.5</sub>. For UFPs, the number of AURN sites in the UK is very limited, and an appropriate background site with available UFPs data is Chilbolton (to inform the modelling background). For NO<sub>2</sub>, and PM<sub>2.5</sub>, the emission inventories were derived based on the UK NAEI emissions at a spatial resolution of 1x1 km<sup>2</sup>. Unlike emission inventories for traditional air pollutants (e.g. NO<sub>2</sub> and PM<sub>2.5</sub>), there are limited sources for the emission inventory for UFPs in the UK. Such an emission inventory for UFPs has been developed by TNO in the RI-Urbans project and the 6 km × 6 km resolution emissions have been used in the Birmingham Pilot modelling study. For the explicit major road emissions, the local traffic model datasets have been obtained from Transport for West Midlands and Birmingham City Council. An Atmospheric Emissions Inventory Toolkit (EMIT developed by Cambridge Environmental Research Consultants, CERC) has been used to pre-process all types of emission sources before these can be used by the ADMS-Urban model. The advanced street canyon and urban canopy module was applied to account for the local street canyon effect for road emissions and spatially varying urban canopy flow for all source types. A novel task farming approach was implemented to enable the parallel running of the same or sequential code with different modelling parameters and inputs on multiple cores on supercomputer clusters at the University of Birmingham. The baseline modelling for the year of 2019 has been evaluated against local air quality measurement sites using a Model Evaluation Toolkit (developed by CERC) with good model performance. The model can generate high resolution air quality maps at 10 m x 10 m, which can be used to investigate spatial and temporal concentration variability.

The ADMS-Urban model was performed for the whole year of 2019. Summer and Winter concentrations can be extracted and compared. Here, Summer represents the months of June, July and August 2019, while Winter is for the months of January, February and December 2019. Figure 3 shows the comparison of Summer and Winter concentrations for NO<sub>2</sub>, PM<sub>2.5</sub>, and PNC. There were relatively higher concentrations of NO<sub>2</sub>, PM<sub>2.5</sub>, and PNC near motorways and major roads in city centre areas, mostly due to the higher traffic-related emissions. This finding was also indicated in the Paris pilot. Away from major roads and in rural areas, concentrations were generally lower. The modelled concentrations of NO<sub>2</sub>, PM<sub>2.5</sub>, and PNC are relatively higher in Winter than these in Summer, which was also found in other pilots. In Winter, the boundary layer height is relatively lower and the atmosphere may have more stable occurrence due to the lower temperature. Also, there might be more activity of residential emissions (e.g. wood burning) in Winter, which will largely contribute to PM concentrations. In Summer, the atmosphere tends to be more unstable due to more surface heating from the sun, which will enhance the local dispersion.

The model performance was evaluated against local measured concentrations obtained from UK AURN and Birmingham Air Quality Supersite (BAQS) using the Model Evaluation Toolkit. These station types are classified as roadside and urban background stations. The Model Evaluation Toolkit calculates statistics from the hourly modelled and measured concentrations. The model evaluation statistics are shown in Tables 7, 8, and 9. for NO<sub>2</sub>, PM<sub>2.5</sub>, and PNC respectively. The measured concentrations were well captured by the model and there are small MFB, i.e. between -15% and 17%. For PNC, MFB is larger between -36% and 30%. MFE outcomes indicate that the modelled concentrations satisfy the strictest performance criteria for NO<sub>2</sub> and PM<sub>2.5</sub>, but less strict performance criteria for PNC. It is noted that there is only one measurement station (from BAQS) with available PNC data for model evaluation. For all pollutants and all station types, RMSE in summer is higher than that in winter. Fac2 (the fraction of modelled data within a factor of 2 of observations) is larger than 76% for NO<sub>2</sub> and PM<sub>2.5</sub>, and larger than 61% for PNC.

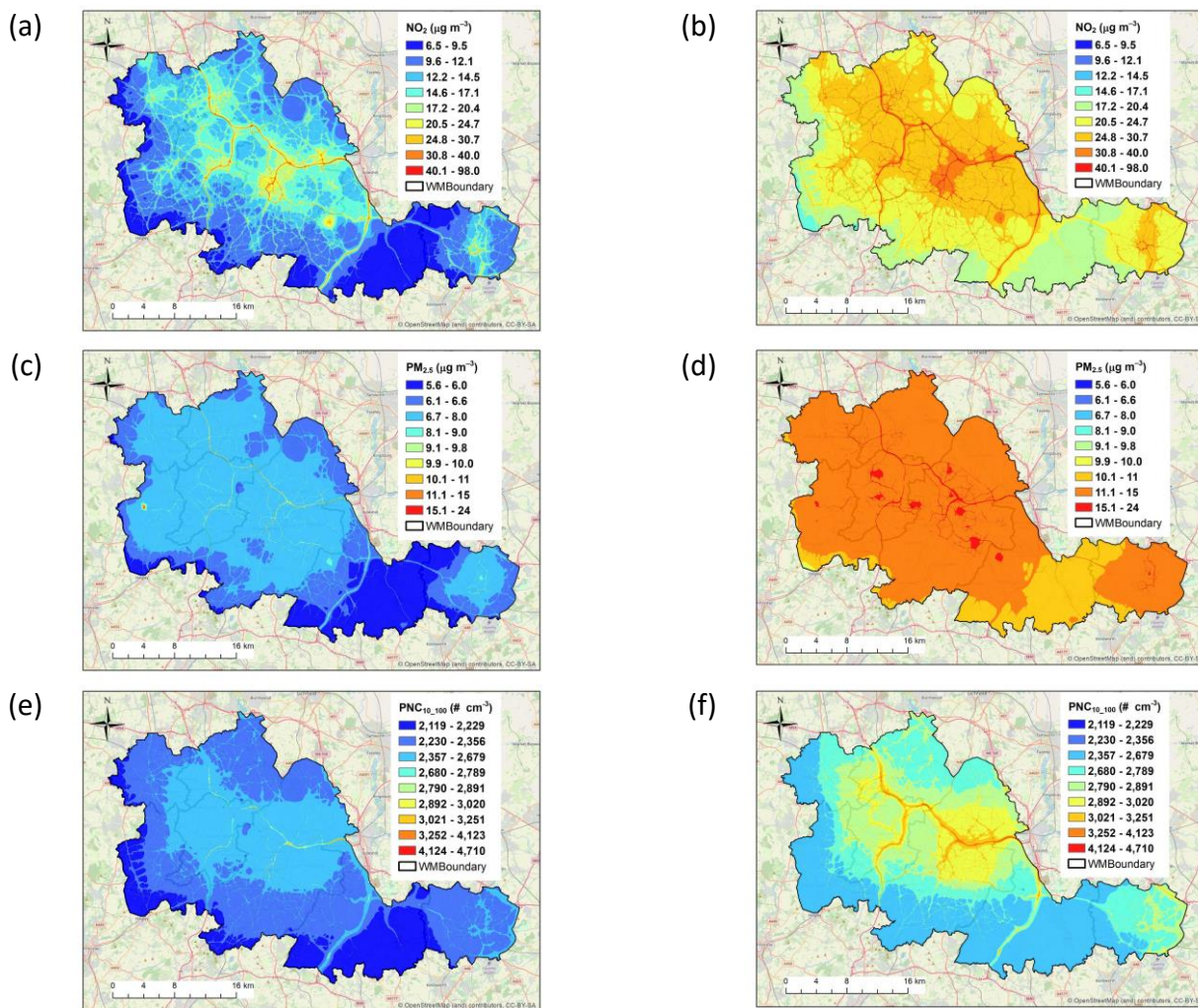


Figure 3. NO<sub>2</sub> [(a) and (b)], PM<sub>2.5</sub> [(c) and (d)], and PNC [(e) and (f)] concentrations simulated for Summer (left panels) and Winter (right panels) using ADMS-Urban.

Table 7. NO<sub>2</sub> model to measurement comparisons at background and roadside stations for Summer and Winter.

NO <sub>2</sub>	Station type	No of stations	Obs (µg m <sup>-3</sup> )	Sim (µg m <sup>-3</sup> )	MFE (%)	MFB (%)	Fac2 (%)
Summer	Roadside	3	25.6	23.6	40	-8	82
	Background	5	12.4	13.7	44	11	77
Winter	Roadside	3	40.4	35.8	40	-15	81
	Background	5	25.0	24.8	41	-0.4	80

Table 8. PM<sub>2.5</sub> model to measurement comparisons at background and roadside stations for Summer and Winter.

PM <sub>2.5</sub>	Station type	No of stations	Obs (µg m <sup>-3</sup> )	Sim (µg m <sup>-3</sup> )	MFE (%)	MFB (%)	Fac2 (%)
Summer	Roadside	1	6.8	7.5	36	14	86
	Background	4	6.6	6.7	37	9	84
Winter	Roadside	1	12.7	14.3	45	17	77
	Background	4	11.7	12.8	46	14	76



**Table 9.** PNC model to measurement comparisons at background and roadside stations for Summer and Winter.

PNC	Station type	No of stations	Obs (# cm <sup>-3</sup> )	Sim (# cm <sup>-3</sup> )	MFE (%)	MFB (%)	Fac2 (%)
Summer	Background	1	3396	2167	59	-36	61
Winter	Background	1	1719	2364	51	30	69

## 6. RECOMMENDATIONS

Urban deterministic models may be used to represent concentrations down to the street scales in cities. Urban variabilities of NO<sub>2</sub>, BC, PNC and PM<sub>2.5</sub> to a lesser extent are particularly large. Spatial variability down to 100x100 m<sup>2</sup> or down to the level of the street segment may be represented, and concentrations may be output hourly or daily, as necessary.

These models require an emission inventory, which can be downscaled from a top-down inventory or correspond to a bottom-up one, and the average characteristics of each main street (height, length and width). For model evaluation, it is advised to evaluate the models at different types of fixed stations characteristic of urban areas (traffic, urban background, suburban background).

In terms of methodology, three different ones are proposed here:

- **Eulerian approach with the CHIMERE/MUNICH/SSH-aerosol chain.** Allowing representation from the regional down to the street scale of NO<sub>2</sub>, PM<sub>2.5</sub>, eBC, PNC as well as of all pollutants that are modelled at the regional scale, as chemistry and aerosol dynamics are modelled at all scales.
- **Hybrid approach (3-D Eulerian grid model with sub-grid Gaussian dispersion) with the EPISODE-CityChem model.** Allowing representation from the regional (1x1 km<sup>2</sup>) down to a 100x100 m<sup>2</sup> scale of NO<sub>2</sub> and PM<sub>2.5</sub>.
- **Gaussian-based approach with the ADMS-Urban model.** Allowing representation down to 10 m<sup>2</sup> scale of NO<sub>2</sub>, PM<sub>2.5</sub> and PNC.

The codes of the models are available at:

- The code of the CHIMERE/MUNICH/SSH-aerosol chain may be obtained from <https://zenodo.org/records/12639507>
- The code of the EPISODE-CityChem model may be obtained from: <https://zenodo.org/records/8063985>
- The code of the ADMS model (for case studies) needs a model licence from Cambridge Environmental Research Consultants <https://www.cerc.co.uk/environmental-software/ADMS-Urban-model.html>

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