Milestone M15 (M3.4)

Improved modelling tools integrating regional and urban scales

RI-URBANS

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

by

FORTH

FOUNDATION FOR RESEARCH AND TECHNOLOGY - HELLAS

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Milestone M15 (M3.4): Improved modelling tools integrating regional and urban scales

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Comments	This document summarizes the first design of the air quality modelling tools integrating regional and urban scales in RI-URBANS. This is the results of the task T3.3 (WP3) on extending AQ modelling to health and policy relevant indicators down to urban scale.

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1. About this document

This document summarizes the first design of the air quality (AQ) modelling tools integrating regional and urban scales in the RI-URBANS project.

This M15 (M3.4) is made in reply to the requirements of WP3-T3.3 on extending AQ modelling to health and policy relevant indicators down to urban scale. This task enhances selected chemistry-transport models (CTMs), PM Comprehensive AQ Model with eXtensions for Ultra-Fine (PMCAMx_UF), CHIMERE (modèle de CHIMie-transport), EMEP-MSC-W model (European Monitoring and Evaluation Programme https://emep.int/mscw), LOTOS-EUROS (LOng Term Ozone Simulation – EURopean Operational Smog model), SILAM (System for Integrated modeLling of Atmospheric coMposition), to quantify source contributions to conventional and novel AQ health metrics (nanoparticles, OP). The CTMs are combined with urban observational data of atmospheric concentrations and 3D profiling and remote sensing (T1.3 and T4.5) to improve modelling scale, vertical information, chemical and microphysical modules for the simulation of nanoparticles (T4.2), PM chemical composition, and VOCs. The improved CTMs capture source contributions of activity sectors and from local sources and long-range transport of PM and nanoparticles. Several modelling strategies are already developed in the Copernicus Atmosphere Monitoring Service (CAMS) Policy Service models: sensitivity simulations, tagging and surrogate modelling and will be confronted to source apportionment products (T1.2). By combining this sectoral information with indicators of OP, oxidative potential (T2.2), more relevant diagnostics for the health-harmful air pollution indicators such as OP are modelled. Maps of source-specific information on health-relevant air pollution indicators at high resolution (1x1 km^2) over specific urban areas and over the remaining European regions will be produced (D3.4). The improved modelling tools will be used in T3.4 and implemented in specific pilot tests-demonstrations (WP4) and in the roadmap for upscaling (WP5).

This is a public document, available in the RI-URBANS website (https://riurbans.eu/work-package-3/#milestones-wp3). The document will be distributed to all RI-URBANS Partners for their use and submitted also to European Commission as the RI-URBANS milestone M15 (M3.4).

2. Emissions

Emission data sets at both regional scales (varying horizontal resolutions from 6 km x 6 km to 36 km x36 km) and urban scales (horizontal resolution 1 km x1 km) modelling studies over the pilot cities will be used in WP3. These are summarized in the next two sections.

2.1. Emissions at the regional scale

TNO has prepared a new pan-European emissions inventory (EI) at a horizontal resolution of 6 km x 6 km. This EI has been described in details in the RI-URBANS M13 (M3.2) report. This is a complete emission dataset for all relevant chemical species. Both the main air pollutants which are also included in CAMS regional inventory, CAMS-REG (CH_4, CO, NH_3, NMVOC, NO_X, SO_2, PM_{10} and $PM_{2.5}$) as well as ultrafine particles (UFP), expressed as particle number (PN) emissions, are included in this inventory.

In terms of emission sectors (SNAP: Selected Nomenclature for reporting of Air Pollutants), road transport exhaust and non-exhaust emissions are covered, but also other relevant sectors for air pollutant emissions. The emissions

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provided in this dataset have a spatial resolution of 6 km x 6 km over the European domain, including the RI-URBANS pilot cities (Figure 1).

This EI will be used as input to the RI-URBANS CTMs operating at regional scales. Depending on the scale, the emissions may be averaged, for example, to the 36 km x 36 km model resolution that will be used by PMCAMx and PMCAMx-UF.

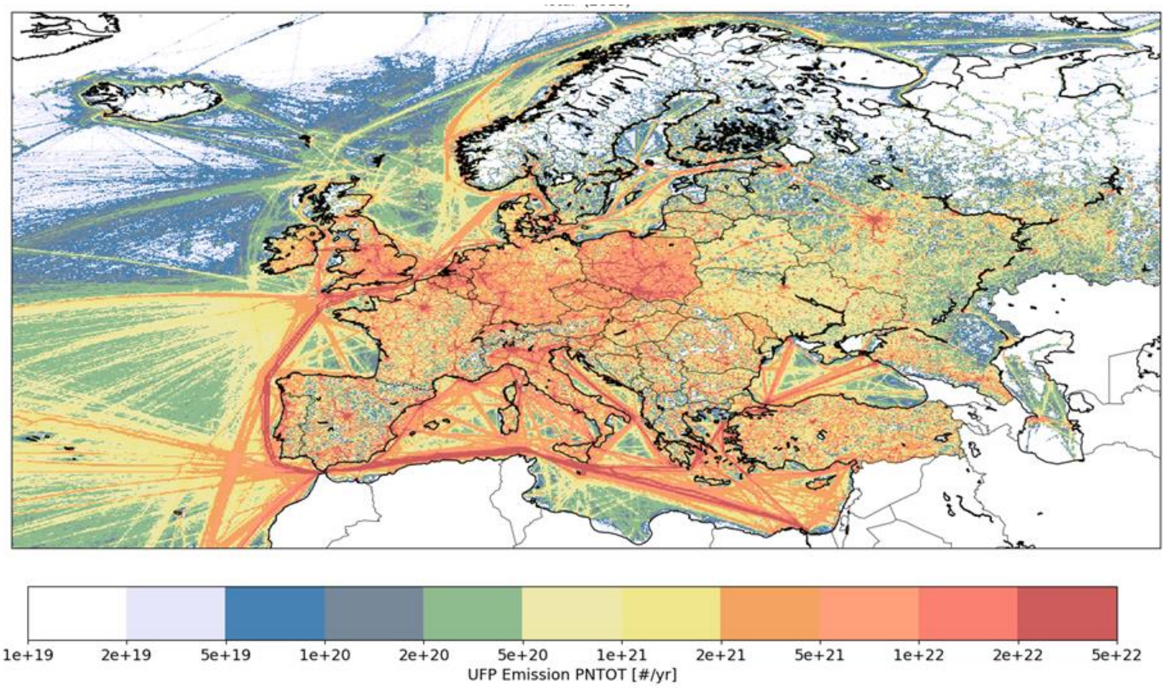

Figure 1. *TNO emissions for particle number for 2018 at 6 km x 6 km spatial resolution.*

2.2. Emissions at the urban scale

High resolution 1km x 1km EIs will be derived for the RI-URBANS pilot cities based on the TNO EI using the downscaling methodology tool developed by NOA and described in the RI-URBANS D17 (D3.2).

In addition, note that for some regions official EIs are available, such as the Dutch national IE which is available also at 1x1 km^2 resolution (Wever et al., 2022).

3. Chemical Transport Modelling

3.1. PMCAMx and PMCAMx-UF

Both PMCAMx and its sister model PMCAMx-UF (focusing on ultrafine particles) will be first applied to the full European modelling domain at a horizontal resolution of 36 km x36 km accepting as inputs the corresponding TNO emissions averaged to this resolution and then the WRF (Weather Research & Forecasting Model) meteorology also averaged at this scale. The two models will then zoom into the pilot cities of interest. Four two-way nests will be used for the dynamic downscaling of the meteorological fields from the outer model domain covering Europe (d01) at 36 km x36 km coarse horizontal resolution down to the 1 km x1 km fine resolution inner domain over the pilot

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city area (d04) (Figure 2). The intermediate model domains d02 and d03, with horizontal resolutions of 12 km x12 km and 3 km x3 km, respectively, will be placed around the d04.

The required meteorological fields will be obtained using WRF v4.1.5 operating at the same spatial resolution as the two CTMs. WRF will be used with 28 vertical sigma levels extending up to a height of approximately 20 km (50 hPa). Biogenic emissions at all scales will be obtained by MEGAN (Model of Emissions of Gases and Aerosols from Nature) model. Details about the approach that will be used by the FORTH team can be found in Siouti et al. (2022).

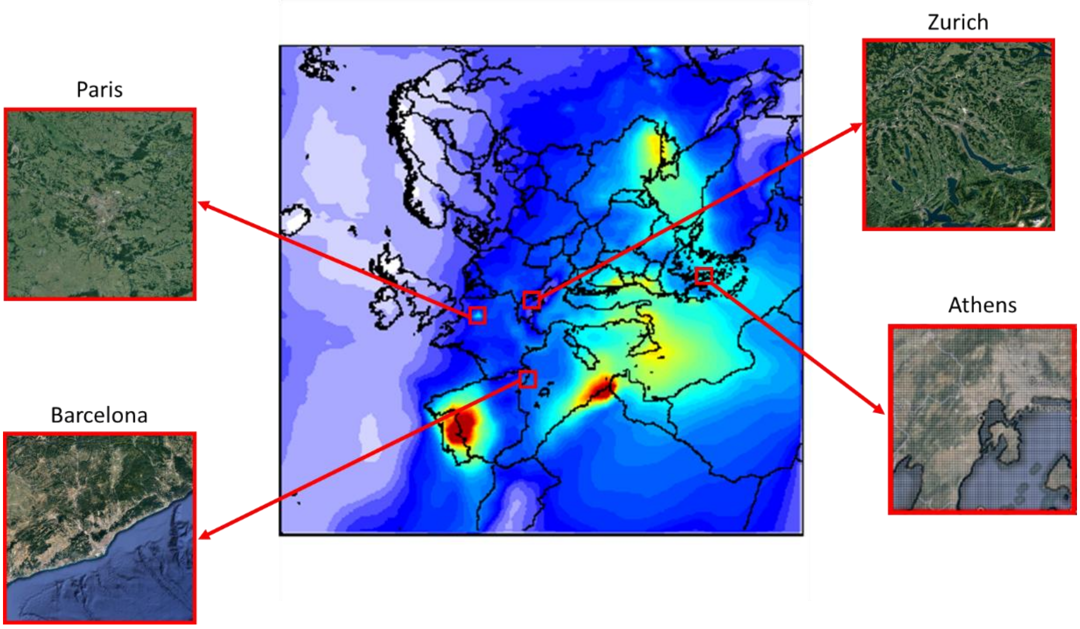

Figure 2. *PMCAMx model domain (d01) at 36 km and the four high resolution domains (d04) over the pilot city areas.*

3.2. CHIMERE

Because of their fundamental role in air pollution, accurate modelling of isoprene (C_5H_8) and elemental carbon (EC) species has become essential for air quality monitoring. CNRS contribution to this RI-URBAN project milestone is to evaluate the surface concentrations of C_5H_8 and EC modelled by regional CTMs over Europe.

CTMs are often routinely compared to standard observations of AQ monitoring networks for chemical species such as PM10, PM2.5, NO_2 and O_3 in the Copernicus Atmosphere Monitoring Service (CAMS). It is however desirable to extend this validation to the more elaborated monitoring developed in supersites such as ACTRIS (Aerosol, Clouds and Trace Gases Research Infrastructure) for species such as VOCs (Volatile Organic Compounds) or PM chemical composition. And such validation raises challenging question regarding the homogeneity and uncertainty of measurement and matching against modelled species. **The validation strategy we are developing in this task, is therefore instrumental to pave the way for service tools making the best use of supersite observation for CAMS modelling applications.**

The CHIMERE model (modèle de CHIMie-transport; https://www.lmd.polytechnique.fr/chimere), together with 7 other CTMs (namely MONARCH, MINNI, MATCH, LOTOS-EUROS, DEHM, EURAD-IM and EMEP) that are part of the CAMS regional production system, are used. The dispersion of responses resulting from the uniqueness of each model gives an idea of the extent of the variability and hence the uncertainty. In addition, simulated concentrations are compared with in situ observations across Europe to assess models' performance.

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A first evaluation was carried out for the year 2018 based on the 8 CTMs on the same simulation domain. The C_5H_8 concentrations were compared with data from 9 measuring stations collected in the EBAS database with atmospheric measurement data. The observed EC concentrations were taken from the RI-URBANS WP1's D1 (D1.1). From these, 13 measuring stations were selected. Promising results emerged from this 2018 test case, as illustrated in Figure 3.

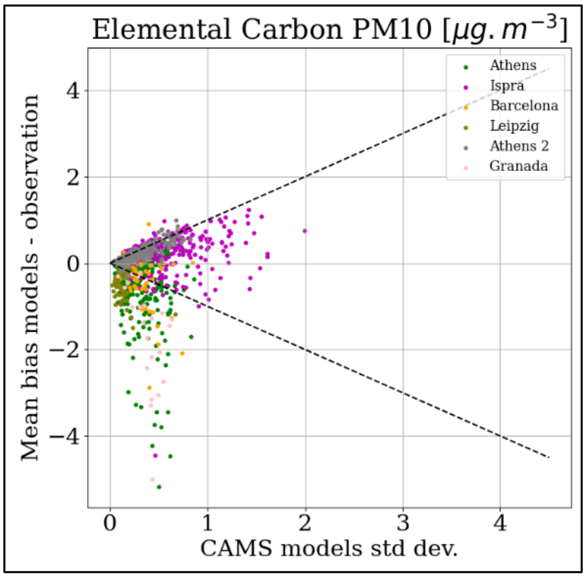

Figure 3. *Preliminary results showing the mean bias (mod. - obs.) of EC (PM_{10}) concentrations and the corresponding standard deviation of the CAMS models for 6 stations.*

Depending on the station analysed, the standard deviation of the CAMS models of the simulated EC can be higher than the average bias (with the corresponding observations), which shows the high variability of the simulated concentrations.

Further work is expected, including a comparison of the PM source apportionment (specifically, the equivalent black carbon, eBC) with observed from recent years. The objective is to provide an operational validation of the CAMS model production system in near-real-time (NRT) at several station points over Europe.

3.3. EMEP and uEMEP

The EMEP MSC-W model will be first applied to the full European domain at a scale of 0.1° x 0.1° (accumulating the TNO emissions to 0.1° x 0.05° (ca 6 km x6 km)). The ECMWF (European Centre for Medium-Range Weather Forecasts) IFS (Integrated Forecasting System) meteorology on the same resolution and domain (0.1° x 0.1°) will be used to drive the EMEP model. The downscaling methodology of the uEMEP model will then be used to zoom into the pilot cities on the desired resolution (at least, 1 km). Details about the uEMEP approach can be found in Denby et al. (2020) and Mu et al. (2022).

The local fraction methodology, a method for e.g., calculating the local source contributions to air pollution (Wind et al., 2020) has been extended to include full chemistry, e.g., different chemical species (and sources) can be included. This method is also the backbone of uEMEP, and will be used here to improve the downscaled results. The local fraction method can also be used to trace different sources, even for organic carbon. This will be important when developing the 'matching' of sources between the model and observations for oxidative potential.

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3.4. LOTOS-EUROS

LOTOS-EUROS (LOng Term Ozone Simulation – EURopean Operational Smog model; https://lotos-euros.tno.nl) will be first applied to the full European modelling domain at a scale of ~25-30 km spatial resolution accepting as inputs the corresponding TNO emissions averaged to this resolution and ECMWF meteorology also averaged at this scale. The model will use 3 or 4 nested domains for downscaling from the outer domain covering Europe at 25-30 km coarse horizontal resolution down to the 1 km fine resolution inner domain over two cities in the Netherlands (Rotterdam and Amsterdam). The intermediate domains, with horizontal resolution 6 km x6 km and possibly 2 km x2 km, will be placed around the city domains. The required meteorological fields will be using ECMWF data.

For the higher resolution model runs we will use either the official national emission inventory and/or the downscaled inventory produced within the RI-URBANS project and seek to implement coupling with meteorological fields from the HARMONIE (HIRLAM ALADIN Research on Meso-scale Operational NWP in Europe; HIRLAM - High Resolution Limited Area Model & ALADIN - *Aire Limitée Adaptation dynamique Développement InterNational*) numerical weather prediction (NWP) model at 2 km x2 km resolution.

Details about the model and its processes and standard input data can be found in Manders et al. (2017).

3.5. SILAM

An interface has been developed to connect SILAM (System for Integrated modeLling of Atmospheric composition; http://silam.fmi.fi) chemistry-transport model with the Large-Eddy Simulation (LES) model PALM (PArallel Large eddy simulation Model; https://palm.muk.uni-hannover.de/trac) of the University of Hannover. The challenge of the interfacing consisted of several conceptual mismatches between underlying assumptions in the models (Table 1).

***Table 1**: Inconsistencies between assumptions in PALM-LES and in SILAM.*

	PALM LES	SILAM
Vertical layers	Given height above the base level	Height above surface or hybrid sigma-pressure
Air density	Constant	Varying with temperature and pressure, pressure varies with height
Temperature, humidity	Constant	3D fields from driving meteorology
Turbulent mixing	Mostly resolved	Fully parameterized
Terrain	Cut cells from the domain	Terrain-following vertical
Horizontal grid	Metric, cartesian	(rotated) Lon-Lat

To match the grids, we have chosen a rotated Lon-Lat grid with the equator going through the centre of the model domain and directed along the longest dimension of the LES grid. The grid points were chosen to match the original LES grid. The LES output was converted to GRIB (GRIdded Binary) format files with the resulting grid and SILAM was instructed to perform the simulations at that grid. With such a setup, boundary conditions can be ingested into SILAM through the same pathway as in any other limited-area simulation.

Since the main equation that SILAM solves is the mass-conservation equation the interfacing was done to maintain the air-mass fluxes through the cell interfaces. Therefore, we adopted the concept of cut-out cells from the driving LES model. The fields of temperature and specific humidity were set constant, and the vertical layers produced by the LES model were redefined for SILAM to match the per-area mass density of air in each level.

The wind speed at cell interfaces within the terrain was forced to zero.

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With such setup we achieved 1:1 match of the SILAM and LES model cells at expense of slightly skewed vertical dimension of the domain. For the simulations the parametrisation of the turbulent mixing in SILAM was disabled to leave only the resolved part of the turbulence. Preliminary tests on a flat terrain domain have shown that such a change although leads to somewhat less mixing in SILAM than with the original LES transport schemes, but still reproduces main statistical properties of the simulated scalar fields.

The interfacing was tested with PALM LES simulations of air flow over the city of Turku (Finland) simulated within a 12x12 km^2 domain with a spatial resolution of 16 m. Preliminary tests with a point source over the Turku domain have shown promising results. The simulated plume looks realistic and does not create any notable artefacts around the cells cut-out due to terrain (Figure 4).

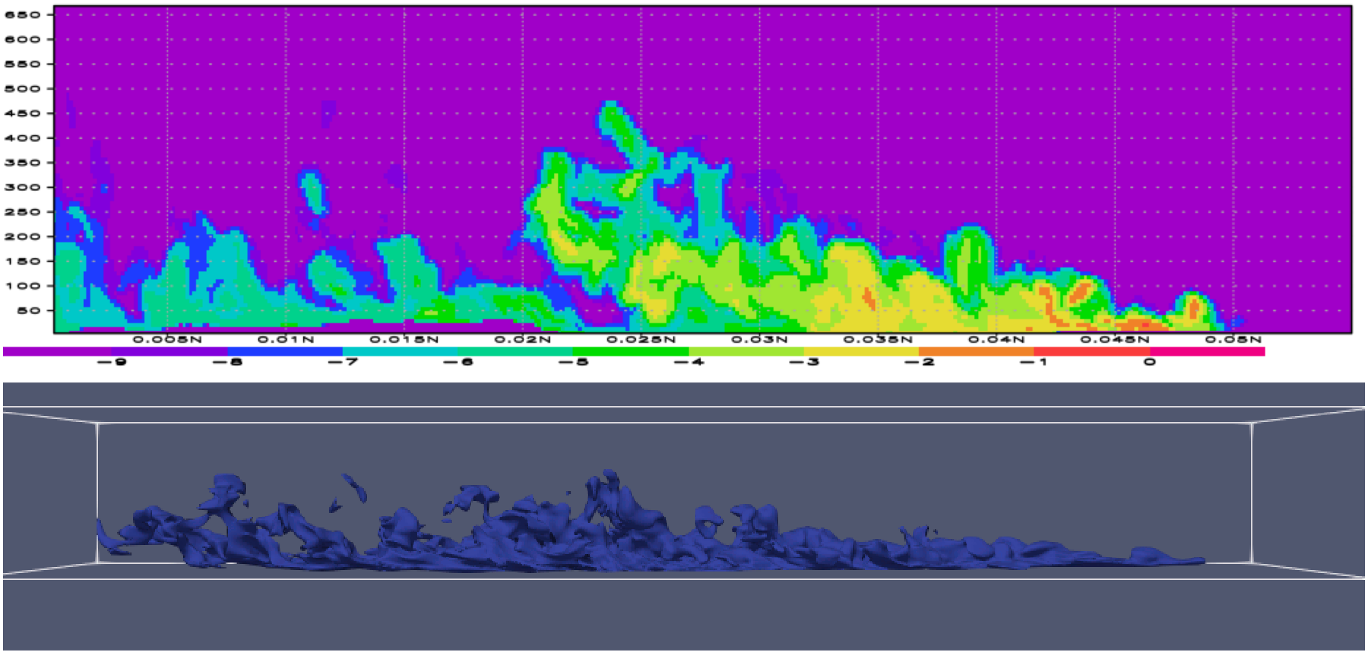

Figure 4. *A snapshot of the passive-tracer simulation from a point source in the Turku harbour. The domain shown is 6km wide and 700m tall. The upper panel shows the decimal logarithm of concentration along a vertical slice of the domain, and the lower panel shows a 3D view of an iso-surface of concentration. The cells cut out by the terrain visible in the bottom of the domain at the upper panel.*

3.6. MONARCH

The MONARCH (Multiscale Online Nonhydrostatic AtmospheRe CHemistry model; https://dust.aemet.es/about-us/monarch) atmospheric chemistry model has been set up by BSC to conduct simulations of black carbon (BC) levels and source contribution in the Spanish Barcelona (urban), Montseny (rural) and Montsec (remote) monitoring sites. A nesting configuration was designed to cover the Barcelona region at 1 km x1 km horizontal resolution with a European parent domain of 20 km x20 km resolution. Emissions from the HERMESv3 (High-Elective Resolution Modelling Emission System) bottom-up emission inventory of T3.1 and the regional European CAMS-REG inventory were used in these respective domains. By using measurements from WP1, both the annual variability of BC in the three sites and the source contribution from residential combustion and traffic sectors have been analysed.

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4. Chemical Transport Modelling at Urban and Street Scales

To represent the heterogeneities of concentrations in cities, the urban concentrations estimated with the CTM of section 3 are downscaled to the street scale. Two approaches are used: a Gaussian approach with the model ADMS (Atmospheric Dispersion Modelling System) (Pilot cities - Birmingham, UK and Paris, France) and a Eulerian approach with the model MUNICH (Pilot city - Paris).

4.1. ADMS

The ADMS-Urban model is used to transport so-called traditional air pollutants (NO_2, PM_{10} and $PM_{2.5}$). The methodology schematics and workflow are described in Figure 5.

This model is used over the Birmingham and Paris urban areas to provide detailed maps on concentrations of traditional air pollutants, see Figure 6 as an example. Note that black carbon will be added in the ADMS-Urban modelling over Paris.

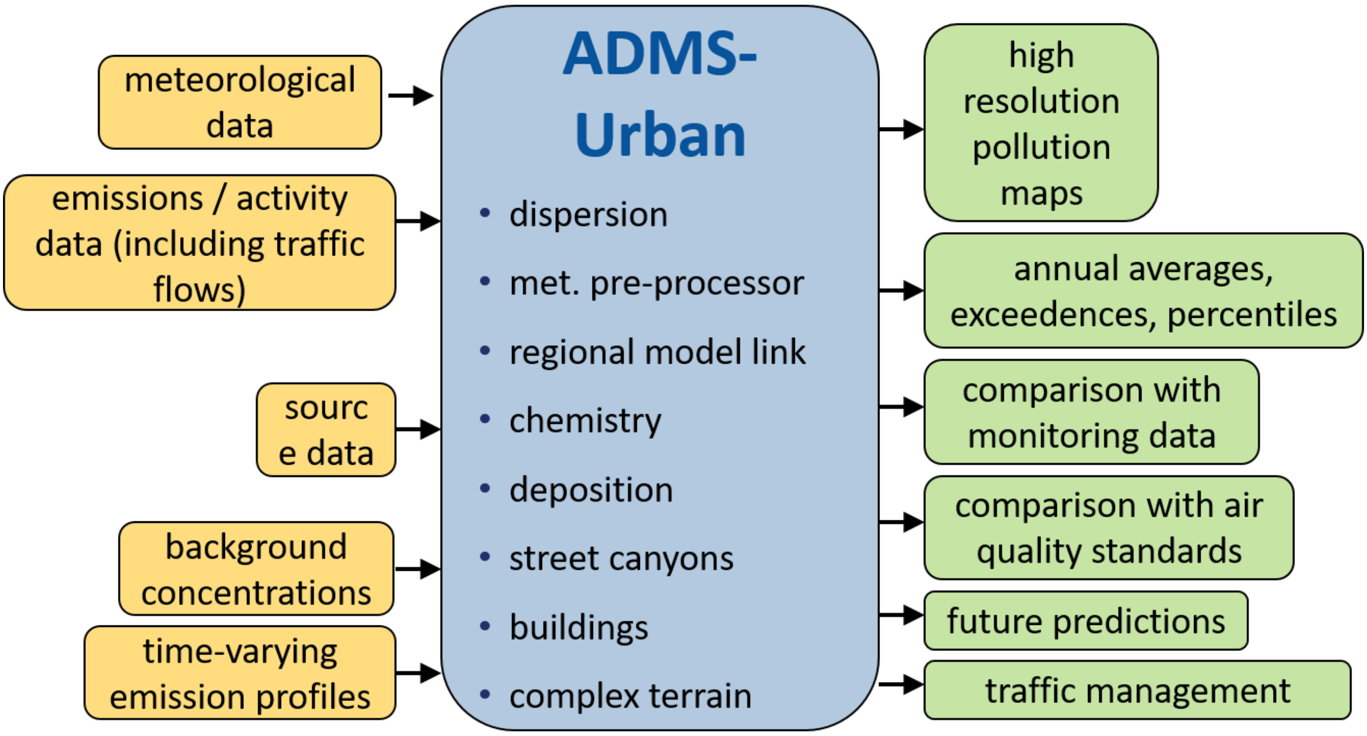

Figure 5. *Description of the ADMS-Urban model.*

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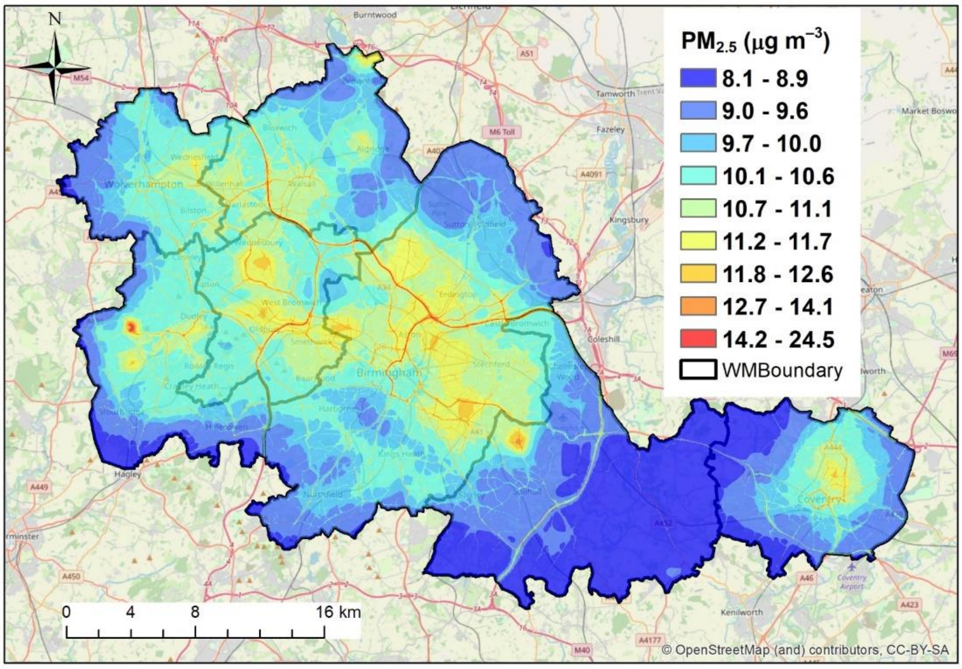

Figure 6. *$PM_{2.5}$ concentrations in 2019 over Birmingham, UK.*

4.2. MUNICH

The MUNICH (The Model of Urban Network of Intersecting Canyons and Highways; http://cerea.enpc.fr/munich) model is a Eulerian model representing the pollutant concentrations in street considering aerosol dynamics, chemistry, transport within street, contribution from the background, and deposition (see description in Figure 7, and Kim et al., 2022). In MUNICH, the aerosol dynamics and chemistry are taken into account by using the SSH-aerosol module (Sartelet et al., 2020). The SSH-aerosol module is based on the coupling of 3 state-of-the-art modules such as SCRAM (Size-Composition Resolved Aerosol Model), SOAP (Secondary Organic Aerosol Processor), and H2O (Hydrophobic/Hydrophilic Organics). It is able to simulate the evolution of gas and particles, including the detailed particle chemistry and ultrafine particles. Over the Paris urban area, MUNICH uses the background concentrations simulated with the regional CTM CHIMERE and the same representation of chemistry and aerosol dynamics as MUNICH. Simulations with the model chain CHIMERE/SSH-aerosol/MUNICH are used in the RI-URBANS pilots to map BC, NO_2, PM, and their detailed composition, as well as UFP-PNC (particle number concentration).

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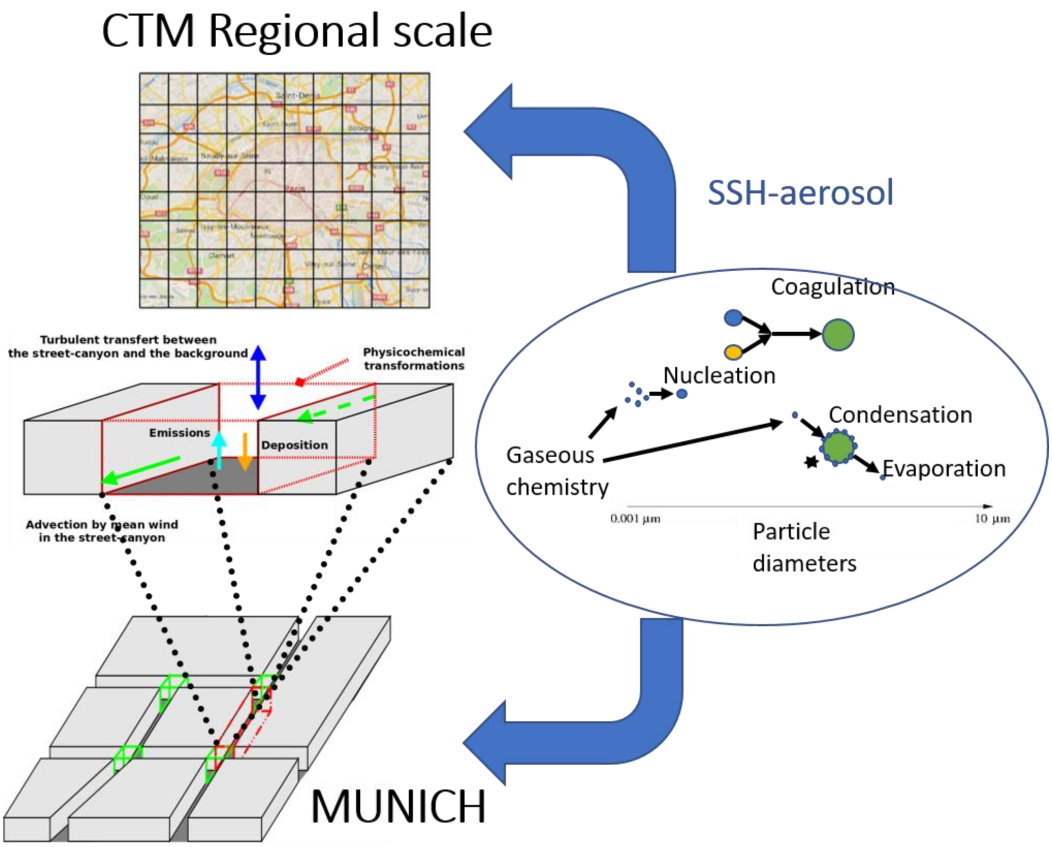

Figure 7. *Description of the modelling with the MUNICH model.*

5. Summary

The RI-URBANS CTMs – PMCAMx/PMCAMx_UF, CHIMERE, EMEP/uEMEP, LOTOS-EUROS, SILAM/PALM, MONARCH - have been modified to allow quantifications of source contributions to conventional and novel AQ health metrics (nanoparticles, OP). Model domains of higher spatial resolution have been set-up centred over the studied cities. Models have been evaluated for their ability to simulate BC observations. Interfaces between the regional models and LES models have been developed to enable realistic simulations of point and city plume dispersion of pollutants. The CTMs at urban and street scales have been set up to use data from the lower resolution CTMs; both the Gaussian (ADMS model) and Eulerian (MUNICH) approaches are used.

In the next phase of the project, the improved CTMs that are able to capture source contributions of activity sectors and from local sources and long-range transport of PM and nanoparticles will be confronted to source apportionment products (T1.2). Using of observationally-derived health indicators' dependences on pollutants from various sectors (T2.2), diagnostics relevant for these health-harmful air pollution indicators such as OP will be calculated. Maps of source-specific information on these indicators at high resolution (1 km x1 km) over specific urban areas and over the remaining European regions will be produced (D3.4).

The improved modelling tools will be then used in T3.4 to assess the efficiency of policy measures at different scales (city, national, EU), building on the new emission inventories (T3.2) and the models' ability to use the novel (ROS, SA information, nanoparticles) and AQ indicators. Furthermore, the modelling tools will be implemented in specific pilot tests-demonstrations (WP4) and in the roadmap for upscaling (WP5).

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