

# LIFEINDEXAIR



## Technical Report on Setup of the Air Modelling System

### Deliverable B3.1

September 2017

THIS PROJECT IS FUNDED BY THE LIFE PROGRAM FROM THE EUROPEAN UNION



**DEMOKRITOS**  
NATIONAL CENTRE FOR SCIENTIFIC RESEARCH



NATIONAL INSTITUTE  
FOR HEALTH AND WELFARE

[WWW.LIFEINDEXAIR.NET](http://WWW.LIFEINDEXAIR.NET)

# CONTENTS

1.	Executive Summary .....	1
2.	Introduction .....	1
3.	Description of the Modelling Setup.....	2
3.1.	Methodology Overview.....	2
3.2.	Definition of Modelling Domains .....	3
3.3.	Input data .....	5
3.4.	Adaptation to the Index-Air Tool .....	6
4.	Conclusions .....	7
5.	REFERENCES .....	8

## 1. EXECUTIVE SUMMARY

The present deliverable describes the modelling setup designed to accomplish the goals of action B3. The main objective of action B3 is to determine the exposure of the target population (children) to the selected pollutants using a modelling approach. A dispersion-exposure modelling system was selected and will be adapted to run in operational mode to allow its use for particulate matter air pollution and exposure control through its integration in the LIFE Index-Air Management Tool.

The report presents the overall modelling methodology, the selected modelling system and its setup for the application to the different Index-Air case studies. Simulation domains and input data required, as well as the methodological approach for the implementation in the Index-Air tool, which is based on neural network training, are also described.

## 2. INTRODUCTION

The Action B3 comprises the compilation of emission data, preparation of meteorological inputs, air quality model setup, and the preparation of the exposure models.

Air quality and human exposure numerical modeling will be used to determine human exposure: first a meteorological model will be applied over the different domains, and then together with emission data, air quality/dispersion simulations will produce the pollutants concentration patterns.

Based on literature and taking into account the expected outputs, the WRF-CAMx air quality modelling system was selected to be applied to the Index-Air urban areas. The WRF model (Weather Research and Forecasting), from the National Center for Atmospheric Research (NCAR) (Skamarock et al., 2008), version 3.5., is a next generation mesoscale numerical weather prediction system designed to serve both operational forecasting and atmospheric research needs. CAMx (Comprehensive Air Quality Model with Extensions) (ENVIRON, 2016) is a 3D chemical transport model suited for the simulations of the emission, dispersion, chemical reactions, and removal of pollutants in the troposphere based on the integration of the continuity equation for each chemical species on a system of nested three-dimensional grids.

The link between emissions and concentrations, described through the WRF-CAMx air quality modelling system, has to be re-written in the context of the Index-Air Management Tool, to be more efficient in terms of CPU demand.

Non-linear models based on Artificial Neural Networks (ANN), similar to the ones presented by Carnevale et al. (2012) and Relvas et al. (2017), can be applied. This approach captures the non-linearity in the relationships between emissions and concentrations, maintaining a low CPU time. Artificial Neural Networks are composed by simple connected elements (neurons) operating in parallel. Each element is characterized through a function (usually nonlinear) relating inputs and outputs (activation function). During the identification phase the weights of the connections between the different neurons are adjusted in order to define a particular function between the network input and output.

### 3.1. METHODOLOGY OVERVIEW

```
graph TD
    EI[Emission Inventory] --> B32
    B31[B3.1 Meteorological Modelling] --> B32
    B32[B3.2 Dispersion Modelling] --> B33
    B33[B3.3 Individual Exposure and Inhaled Dose] --> B34[B3.4 Population Exposure]
    C[Census data] --> B34
    B32 --> B34
```

The flowchart illustrates the B3 Exposure Assessment Framework, which integrates various data sources to assess population exposure. The process begins with the **Emission Inventory** (Gridded emissions by SNAP macrosector for gaseous and particulate pollutants, 1x1 km<sup>2</sup>) and **B3.1 Meteorological Modelling** (3D meteorological fields from WRF). These inputs feed into **B3.2 Dispersion Modelling** (CAMx), which produces surface gridded concentrations by PM species (1h, 1x1 km<sup>2</sup>). This output, along with **Census data**, feeds into **B3.4 Population Exposure**. Additionally, **B3.2** interacts with the **B2 AQ database** (Outdoor conc measured, Indoor conc measured, Time-activity patterns) and **B3.3 Individual Exposure and Inhaled Dose**, which also receives **Ventilation rates** and feeds into **B3.4**.

Figure 1 shows the interactions between the different tasks (sub-actions) of Action B3, the outputs of each one that will be inputs to the subsequent ones and the link to Action B2.

The WRF-CAMx application, with high spatial (~1x1 km<sup>2</sup>) and temporal (1 hour) resolution, will produce the concentration fields over the study regions needed for population exposure estimation. Indoor/outdoor ratios will also be derived making use of data from B2 and used in the individual exposure model.

### 3.2. DEFINITION OF MODELLING DOMAINS

The air quality modelling system will be applied for the 5 Index-Air case studies following a downscaling approach, over three nested domains until reaching the final desired horizontal resolution of 1 km<sup>2</sup> over each urban area. For this purpose, an European domain and 5 regional and urban domains were defined as summarized in Table 1 and displayed in Figure 2 and Figure 3.

Table 1. Air quality modelling domains (European, regional and urban) for the Index-Air study areas.

	European domain	Regional domain	Urban domain
Lisbon, PT		Orig (lon,lat)=(-10.80°,36.20°) 97x127 grid cells ~5x5 km <sup>2</sup>	Orig (lon,lat)= (-9.51°,38.49°) 52x52 grid cells ~1x1 km <sup>2</sup>
Porto, PT			Orig (lon,lat)= (-9.01°,40.99°) 52x52 grid cells ~1x1 km <sup>2</sup>
Kuopio, FIN	Orig(lon,lat)= (-12.5°,35°) 170x116 grid cells ~ 25x25 km <sup>2</sup>	Orig (lon,lat)=(26.95°,62.20°) 27x27 grid cells ~5x5 km <sup>2</sup>	Orig (lon,lat)= (27.49°,62.74°) 27x27 grid cells ~1x1 km <sup>2</sup>
Athens, GR		Orig (lon,lat)=(22.70°,36.95°) 42x42 grid cells ~5x5 km <sup>2</sup>	Orig (lon,lat)= (23.49°,37.74°) 52x52 grid cells ~1x1 km <sup>2</sup>
Treviso, IT		Orig (lon,lat)=(11.20°,44.45°) 42x42 grid cells ~5x5 km <sup>2</sup>	Orig (lon,lat)= (11.99°,45.24°) 52x52 grid cells ~1x1 km <sup>2</sup>

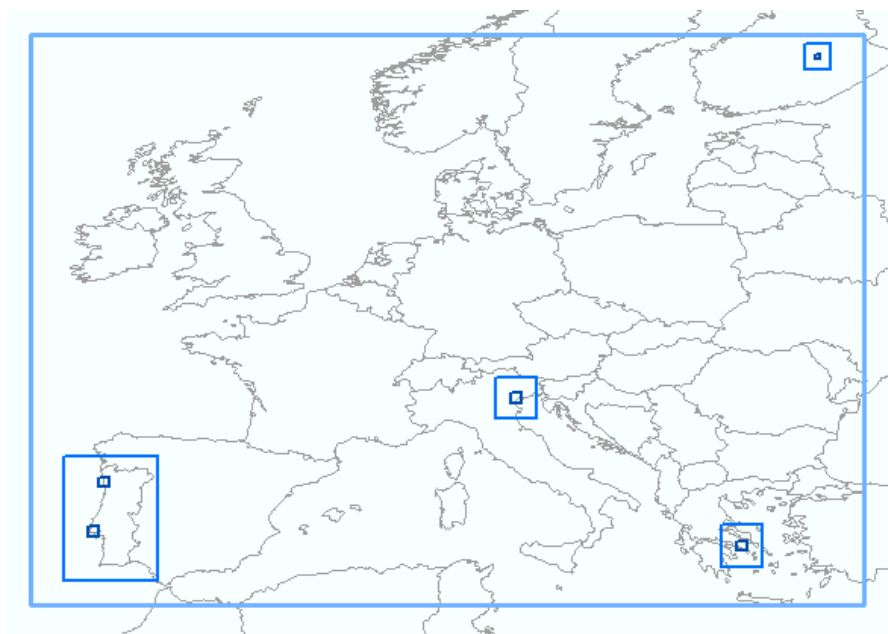
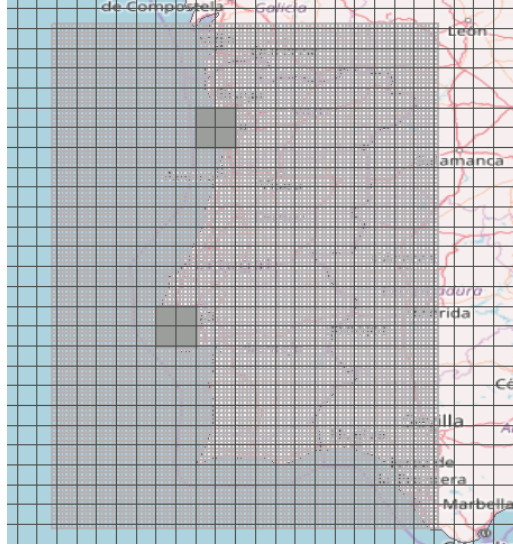
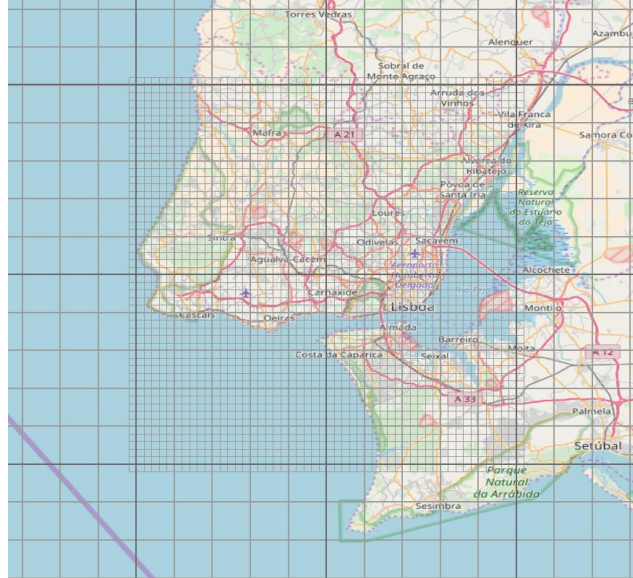


Figure 2. European simulation domain with the location of regional and urban domains for the case studies of Lisbon, Porto, Athens, Treviso and Kuopio.

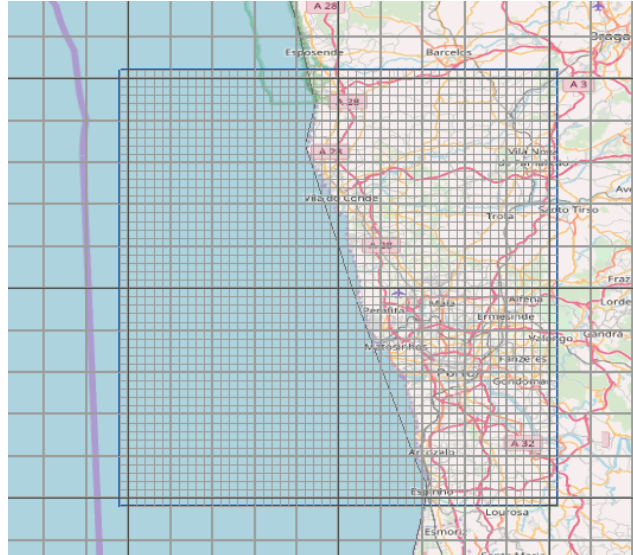
Regional domain for Lisbon and Porto



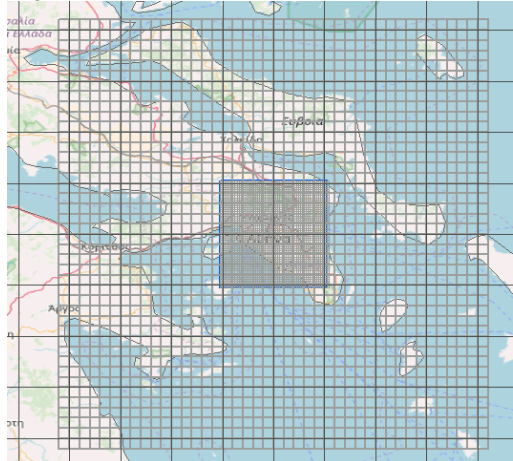
Urban Domain Lisbon



Urban Domain Porto



Regional domain for Athens



Urban domain Athens



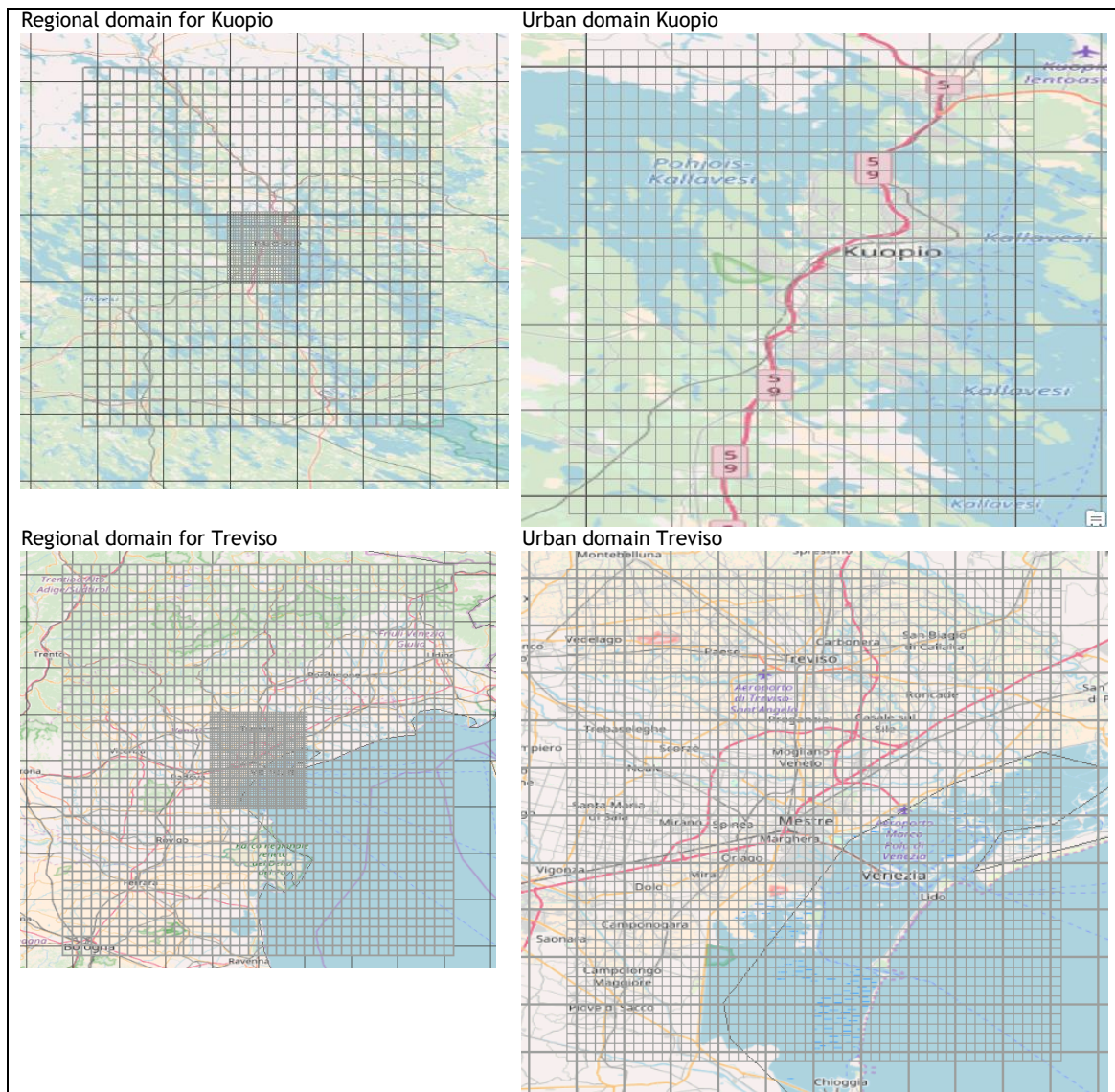


Figure 3. Regional and urban simulation domains for the case studies of Lisbon, Porto, Athens, Treviso and Kuopio.

### 3.3. INPUT DATA

For the application of the air quality and exposure modelling system several types of input data are needed:

- Meteorological data and background concentrations of air pollutants to initialize the WRF and CAMx models, respectively;
- Emission data;
- Air quality measurements (indoor and outdoor) for validation and to compute indoor/outdoor ratios;
- Time activity patterns and ventilation rates of the children under study, for individual exposure modelling;
- Census data for population exposure modelling.

Data needed for the air quality modelling application have been already compiled. Meteorological inputs to the chemical simulations were driven by the meteorological

model WRF, forced by ERA Interim reanalysis data from ECMWF (European Centre for Medium Range Weather Forecast) at 6 hours and 0.75 degrees temporal and spatial resolution, respectively. Initial and boundary conditions for the first domain are provided by the global chemical model MOZART (Emmons et al., 2010) with a time resolution of 6 hours. Anthropogenic emissions were taken from the most recent European emission inventory based on Member States submissions for the year 2015. The EMEP inventory, with an horizontal resolution of 0.1 degrees (approximately 10km), comprises annual emission totals by activity sector for gases and particulate species including metals, was disaggregated to the case study modelling domains and speciated into the CB6 chemical mechanism gaseous species and into the default particulate species considered by CAMx. The chemical mechanism description and treatment was adapted to additionally include the metal species as inert particles.

### 3.4. ADAPTATION TO THE INDEX-AIR TOOL

Air quality modelling simulations by means of WRF-CAMx cannot directly be used inside the Index-Air management tool to simulate the link between precursor emissions and air quality indexes due to their computational time. Aiming to integrate the air quality and exposure components in the tool a new approach was defined.

Artificial Neural Networks (ANN) will be used to simulate the nonlinear source-receptor relationship between concentrations and the emission of precursors. To identify ANN it is first necessary to select the model type, architecture and an input shape adequate to the domain under study and, then, to identify a set of emission-concentration scenarios, that need to be simulated using WRF-CAMx.

When figuring out the most suitable input shape it is assumed that the air quality index (AQI) (e.g. annual mean PM10 concentration) values in a given cell can also depend on the precursor emissions in distant cells. A second key factor, to be taken into account, concerns dominant wind directions. A technique already presented in literature (Carnevale et al., 2012) allows considering these two relevant aspects by aggregating the emissions from cells belonging to four triangular slices, located around the cell for which the AQI has to be computed (Figure 4).

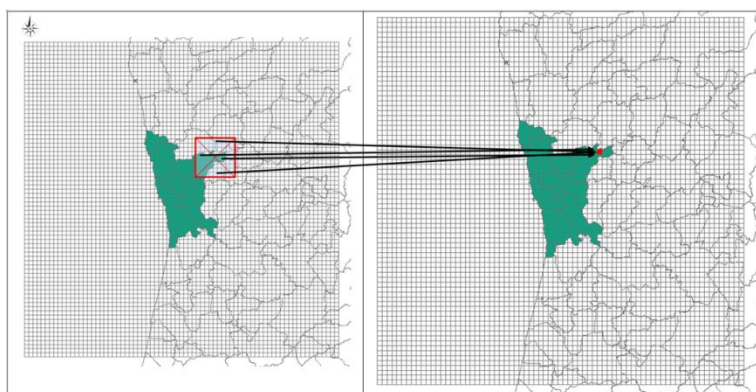


Figure 4. Example of ANN input and output values considering each quadrant.

This configuration has the advantage of being adjustable to different conditions by modifying the dimensions of the quadrants.

After defining the input shapes, for the 5 Index-Air cities, a minimum set of WRF-CAMx simulations is required to provide data for the ANN calibration and validation. Given the high flexibility of the surrogate model structure adopted in this work (feed-forward

neural network), and based on previous works, we estimate that a series of 10 emission reduction scenarios allows identifying the ANN parameters with sufficient accuracy. This minimum number of scenarios has to reproduce all the possible precursor emissions variations. Table 2 presents the list of reduction scenarios that are going to be used to train ANN for the 5 cities.

Table 2. List of the emission reduction scenarios obtained combining B, H, L scenarios.

Scenarios	Urban area emissions			
	NO <sub>x</sub>	VOC	PM	SO <sub>2</sub>
0	B	B	B	B
1	L	L	L	L
2	H	H	H	H
3	H	L	L	L
4	L	H	L	L
5	L	L	H	L
6	L	L	L	H
7	H	H	L	L
8	H	L	H	H
9	H	L	L	H

In order to determine the emission reduction scenarios for which the WRF-CAMx is executed, three levels: B (base case), L (low emission reductions) and H (high emission reductions) will be considered. The B case considers the emissions in 2015 increased by 15% (upper bound) to enlarge the identification bounds for ANN and therefore guaranteeing the correct identification of surrogate models. The H case is associated to the Maximum Feasible Reduction of emissions at 2015 decreased by 15% (lower bound). The L case is an average of H and B. The 15% increase/decrease of emissions is needed in order to train the networks on a wider emission range, avoiding its application with inputs that are too close to the extremes, which could generate boundary effects.

Finally, after training, the trained ANN will be uploaded in the Index-Air tool (as a .csv file) allowing a quick estimation of air pollutant concentrations values based on a variation on precursor emissions, for each one of the 5 cities.

## 4. CONCLUSIONS

The present Deliverable describes the overall modelling methodology. The WRF-CAMx air quality modelling system was selected and its setup for the application to the different Index-Air case studies was defined. The simulation domains and required input data are presented, as well as the methodological approach for the implementation in the Index-Air tool.

## 5. REFERENCES

- Carnevale, C., Finzi, G., Guariso, G., Pisoni, E., & Volta, M. (2012). Surrogate models to compute optimal air quality planning policies at a regional scale. *Environ. Model. Softw.*, 34, 44-50. doi: 10.1016/j.envsoft.2011.04.007
- Emmons, L.K., et al. Description and evaluation of the Model for Ozone and Related chemical Tracers, version 4 (MOZART-4). *Geoscientific Model Development*, 3, pp. 43–67, 2010.
- ENVIRON. User's Guide Comprehensive Air Quality Model with Extensions Version 6.30. Ramboll Environ, Novato, California, 2016.
- Relvas, H., Miranda, A. I., Carnevale, C., Maffei, G., Turrini, E., & Volta, M. (2017). Optimal air quality policies and health: a multi-objective nonlinear approach. [journal article]. *Environmental Science and Pollution Research*, 1-13. doi: 10.1007/s11356-017-8895-7
- Skamarock, W.C., et al. A Description of the Advanced Research WRF Version 3. NCAR/TN-475+STR Ncar Technical Note. 2008.