

# LJUBLJANA

## MESOSCALE AIR QUALITY ANALYSIS

### 1. MODELLING APPLICATION

This report provides an overview of the modelling approach used to characterize the air quality in the Ljubljana region, which includes a detailed description of the air quality modelling system WRF-CAMx (section 1.1.) and a description of the methodology applied to evaluate the model performance (section 1.2.)

#### 1.1. Air quality assessment

The CAMx - Comprehensive Air Quality Model with Extensions<sup>1</sup>, forced by the WRF - Weather Research and Forecasting<sup>2</sup> meteorological fields, was applied over Ljubljana region for the year of 2010, the base year for ClairCity project. The CAMx Particulate Source Apportionment Technology (PSAT) was applied to quantify the contributions of multiple source areas, categories, and pollutant types to ambient pollution, over the case study region.

The WRF model, from the National Center for Atmospheric Research (NCAR), version 3.7., is a next generation mesoscale numerical weather prediction system designed to serve both operational forecasting and atmospheric research needs. CAMx is a 3D chemistry-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 gas-phase photochemistry is resolved through the Carbon Bond (CB05 or CB6) or the SAPRC99 chemical mechanism. CAMx includes a source apportionment (SA) or attribution capability that chemically apportions PM<sub>10</sub>, PM<sub>2.5</sub> and NO<sub>2</sub> to boundary conditions and emissions. This approach estimates the contributions from multiple source areas, categories, and pollutant types to the spatial and temporal distribution of the pollutants concentrations in a single model run<sup>3</sup>.

CAMx version 6.30, with its PSAT tool, was applied over case study region using a two-nesting approach based on a European domain with 0.25 degrees' horizontal resolution and the domain of interest centred in Ljubljana, with 35 by 30 cells, at 0.05 degrees' horizontal resolution (Fig. 1). 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 provided by the global chemical model MOZART<sup>4</sup> with a time resolution of 6 hours. Anthropogenic emissions for both domains were taken from the TNO-MACC\_II European emission inventory<sup>5</sup> available at a resolution of 0.125 by 0.0625 degrees and were speciated into the CB6 chemical mechanism species considered in the CAMx simulation<sup>6</sup>.

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<sup>1</sup> ENVIRON (2016) User's Guide Comprehensive Air Quality Model with Extensions Version 6.30. Novato, California

<sup>2</sup> Skamarock WC, Klemp JB, Dudhia J, et al (2008) A Description of the Advanced Research WRF Version 3 NCAR/TN-475+STR. Boulder, Colorado, USA

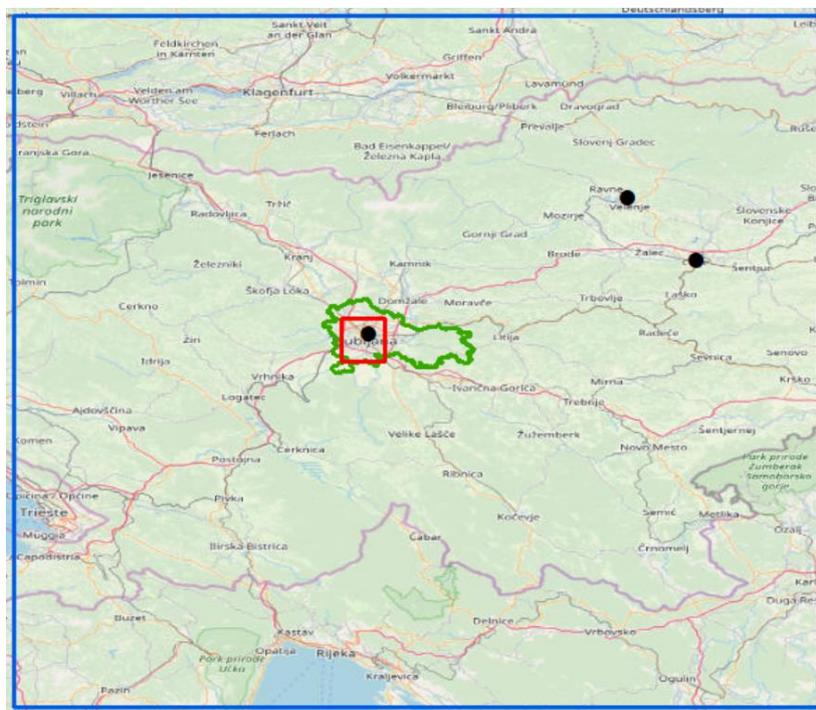
<sup>3</sup> Yarwood G, Morris RE, Wilson GM (2007) Particulate Matter Source Apportionment Technology (PSAT) in the CAMx Photochemical Grid Model. In: Borrego C, Norman A-L (eds) Air Pollution Modeling and Its Application XVII. Springer, Boston, pp 478–492

<sup>4</sup> Emmons LK, Walters S, Hess PG, et al (2010) Description and evaluation of the Model for Ozone and Related chemical Tracers, version 4 (MOZART-4). *Geosci Model Dev* 3:43–67. doi: 10.5194/gmd-3-43-2010

<sup>5</sup> Kuenen JJP, Visschedijk AJH, Jozwicka M, Denier van der Gon HAC (2014) TNO-MACC\_II emission inventory; a multi-year (2003-2009) consistent high-resolution European emission inventory for air quality modelling. *Atmos Chem Phys* 14:10963–10976. doi: 10.5194/acp-14-10963-2014

<sup>6</sup> Yarwood G, Jung J, Whitten GZ, et al (2010) Updates to the carbon bond mechanism for version 6 (CB6). In: 9th Annual CMAS Conference. Chapel Hill, NC

The PSAT application requires the definition of source groups to be tracked and thus the input of extra emission files for each of the groups to be considered. Based on the Slovenia national emission inventory<sup>7</sup> and on the emission sources, the main sectors contributing to PM<sub>10</sub>, PM<sub>2.5</sub> and NO<sub>2</sub> emissions in the year under study (2010) are: (i) residential and commercial combustion; (ii) road transport; and (iii) industry. In this sense, emissions were splitted into these activity sectors in order to evaluate the individual contribution of each source sector to the air quality in Ljubljana urban area (the receptor area considered for source apportionment) through the PSAT application.



**Figure 1** – Blue square - CAMx nested domain with 0.05° horizontal resolution. Green contour - Ljubljana municipality area. Black points – Ljubljana Bežigrad, Celje and Skale urban background air quality monitoring stations, used to evaluate the model performance. Red square - urban area considered in the SA application.

## 1.2. Model evaluation

The model system performance was evaluated through a statistical analysis. The following statistical parameters were computed:

- **Fractional Bias (FB)**: is normalized by the mean of the observed and modelled values. This modified mean bias ranges between -2 and 2. The closer to 0 the value, the better the model. The FB is unitless.
- **Root Mean Square Error (RMSE)**: measures the standard deviation of the differences between the modelled and the observed values. It is the most common estimator of the accuracy of the model system. The closer to 0 is the RMSE, the better the model system performance. The RMSE is given in  $\mu\text{g}\cdot\text{m}^{-3}$ .
- **Correlation (r)**: refers to the extent to which the modelled and the observed values have a linear relationship with each other; the correlation is comprised between -1 and 1. The closer to 1, the better the model system performance. The r is unitless.

A perfect model would have B, FB and RMSE equal to 0.0 and r equal to 1.0

<sup>7</sup> Logar, M., et al. (2018) Informative Inventory Report Slovenia 2018. Slovenian Environment Agency

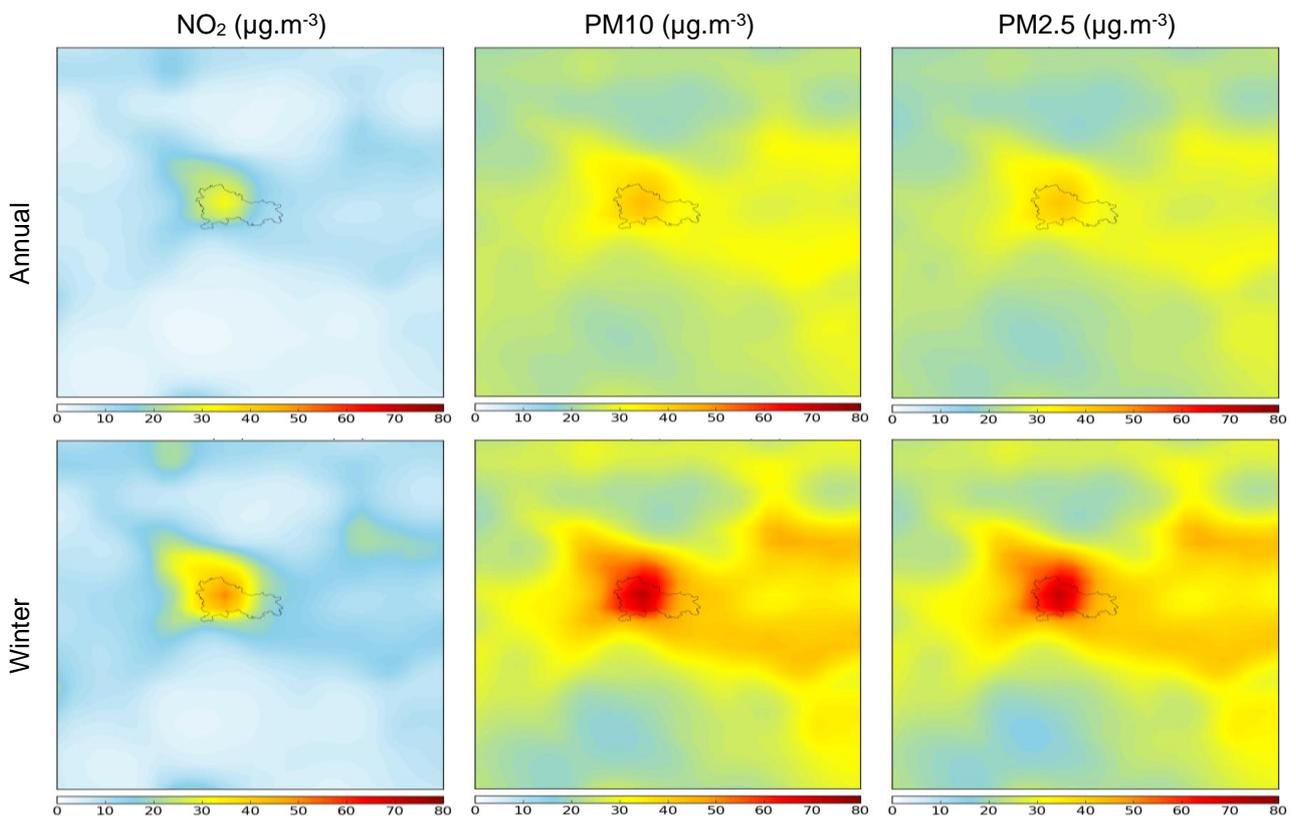
## 2. ANALYSIS OF RESULTS

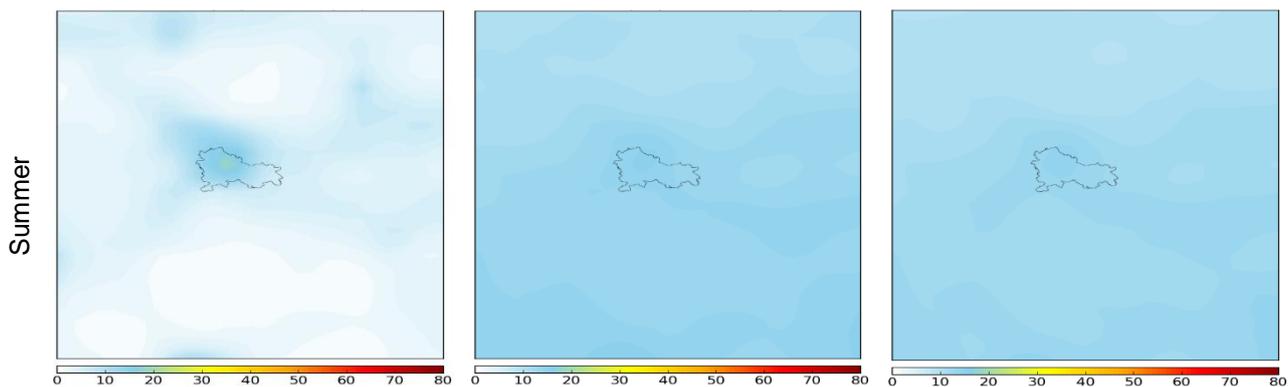
### 2.1. Air quality assessment

The air quality characterization in the Ljubljana region was based on spatial maps of concentrations (section 2.1.1) and on a source contribution analysis (section 2.1.2). The spatial analysis was done for the average concentrations of NO<sub>2</sub>, PM<sub>10</sub> and PM<sub>2.5</sub> for the following periods: (i) annual; (ii) a typical winter month (February); and (iii) a typical summer month (August). The source contribution analysis was provided to estimate the contribution to the modelled PM<sub>10</sub>, PM<sub>2.5</sub> and NO<sub>2</sub> concentrations, from transboundary transport (TBD) and from specific source groups previously defined – residential and commercial combustion (RES), industrial combustion and processes (IND), road transport (TRP) and all the remaining sources (OTH). The results were analysed in terms of the relative contribution of those groups to the PM<sub>10</sub>, PM<sub>2.5</sub> and NO<sub>2</sub> concentration simulated for the urban area of Ljubljana (URB) which was the receptor area defined in the PSAT application (see Fig. 2).

#### 2.1.1. Concentration Fields

Fig. 2 presents the NO<sub>2</sub>, PM<sub>10</sub> and PM<sub>2.5</sub> concentration fields obtained by the WRF-CAMx application for the tree periods previously defined. Results show similar spatial patterns for the different periods and pollutants analysed. For all pollutants, the highest concentration values are found in Ljubljana municipality area.

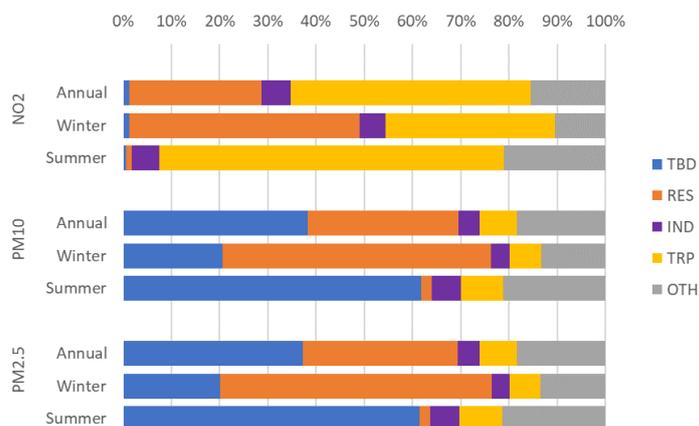




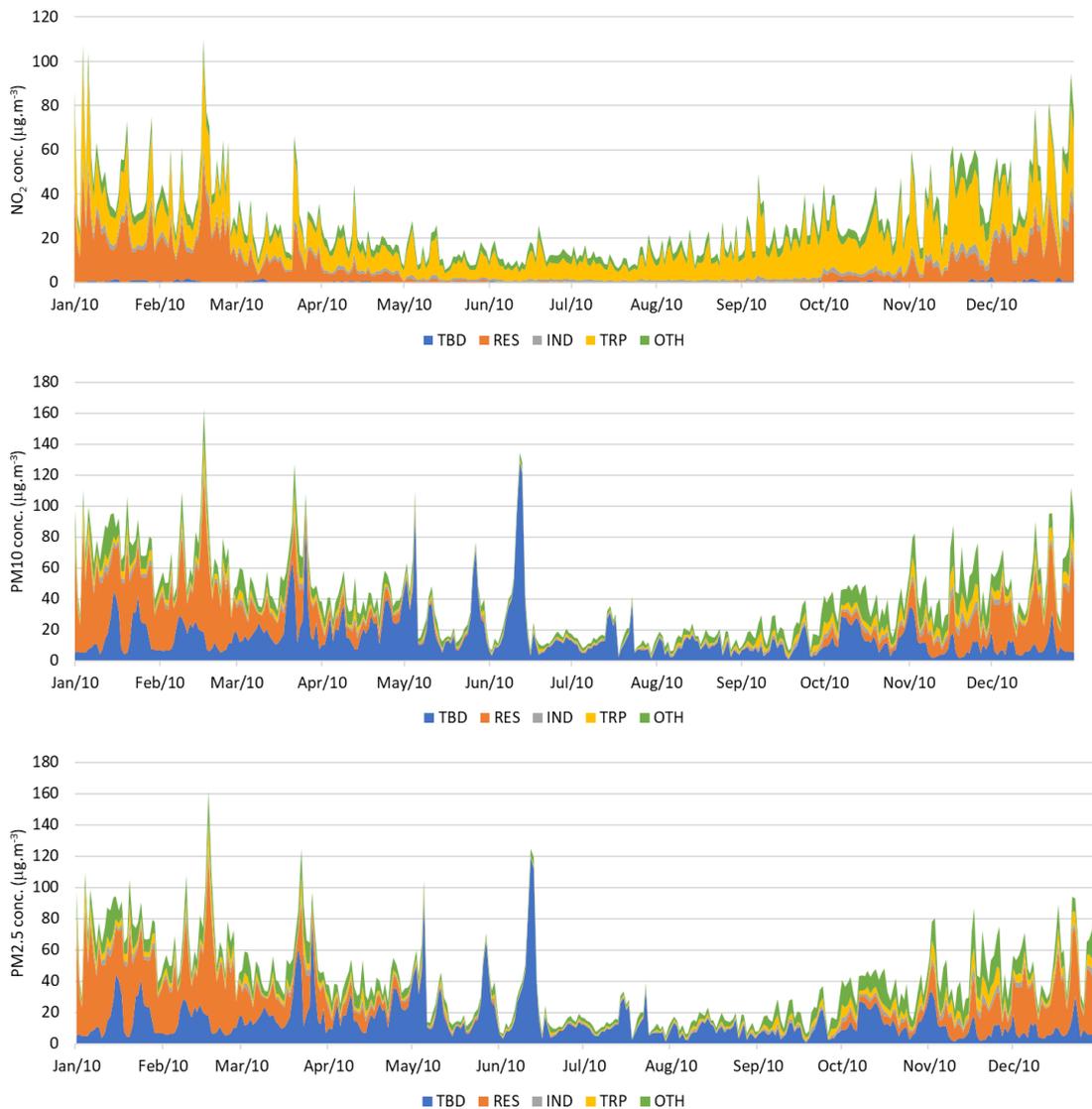
**Figure 2** - Spatial distribution of NO<sub>2</sub>, PM<sub>10</sub> and PM<sub>2.5</sub> concentrations.

### 2.1.2. Source contribution analysis

The contribution of each source group for PM<sub>10</sub>, PM<sub>2.5</sub> and NO<sub>2</sub> concentrations, in the URB receptor for the three periods previously defined, are analysed in Fig 3. Fig. 4 shows the time series of daily average contributions for each source group for PM<sub>10</sub>, PM<sub>2.5</sub> and NO<sub>2</sub> concentrations, for the entire year of 2010.



**Figure 3** – Annual, winter and summer averages contribution for each source group for PM<sub>10</sub>, PM<sub>2.5</sub> and NO<sub>2</sub> concentrations.



**Figure 4** – Time series of daily average contributions for each source group for NO<sub>2</sub>, PM10 and PM2.5 concentrations.

For NO<sub>2</sub>, the annual average contributions of each source group reveal that the major contribution is from road transport, with values around 50%. In the winter period, the contribution of residential and commercial combustion increases, with values up to 45%. On the other hand, during summer, the contribution of residential and commercial combustion is quite small, with road transport having a contribution of about 70%. The annual average contributions of each source group reveal that one of the major contributions is from TBD (38% for PM10 and 37% for PM2.5), highlighting the importance of transboundary transport for the PM pollution in the study region. This background/transboundary effect is even more notorious in the summer period, with values of 62%. Source contribution results also point to a great influence of the contribution of different human activities, such as residential and commercial combustion and road transport, to the PM levels, with the residential commercial combustion being higher in the winter period and the road transport in the summer period.

Although the other sources (OTH) have a significant contribution for NO<sub>2</sub>, PM10 and PM2.5 concentrations, in this analysis it is neglected, as it represents several groups, rather than a specific source group.

## 2.2. Model evaluation

In order to evaluate the performance of the WRF-CAMx modelling system, a set of statistical metrics were estimated (Table 1), considering the Celje, Ljubljana Bezigrad and Skale urban background air quality monitoring stations observed data as reference values. For this analysis, hourly data was considered, for the entire year of 2010 and taking into account the station's monitoring efficiency.

**Table 1** - Statistical analysis of the WRF-CAMx model system, for Celje, Ljubljana Bezigrad and Skale air quality monitoring stations, considering the observed data as reference.

<b>Air quality station</b>	<b>Pollutants measured</b>	<b>Station efficiency (%)</b>	<b>FB (-)</b>	<b>RMSE (<math>\mu\text{g.m}^{-3}</math>)</b>	<b>r (-)</b>
Celje	PM10	96.24	-0.01	26.80	0.39
Celje	NO <sub>2</sub>	93.61	-0.67	21.41	0.45
Ljubljana Bezigrad	PM10	95.30	0.29	36.45	0.41
Ljubljana Bezigrad	NO <sub>2</sub>	93.72	-0.19	27.22	0.49
Skale	PM10	95.07	0.11	19.42	0.45
Skale	NO <sub>2</sub>	92.44	0.46	9.76	0.37

In average, the RMSE, the standard deviation of the differences between the modelled and the observed values, is between 10 and 37  $\mu\text{g.m}^{-3}$ , and the correlation between modelled and observed values is higher than 37%. For FB, negative values are obtained for both pollutants in Celje and for NO<sub>2</sub> in Ljubljana Bezigrad, showing an underestimation of the model results, compared with the observed values. For the other cases an overestimation of the model results is observed.