

AVEIRO REGION

MESOSCALE AIR QUALITY ANALYSIS

1. MODELLING APPLICATION

This report provides an overview of the modelling approach used to characterize the air quality in the Aveiro 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 Extensions¹, forced by the WRF - Weather Research and Forecasting² meteorological fields, was applied over the Aveiro 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 PM₁₀, PM_{2.5} and NO₂ 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 run³.

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 Aveiro Region, with 95 by 125 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 MOZART⁴ with a time resolution of 6 hours. Anthropogenic emissions for both domains were taken from the TNO-MACC_II European emission inventory⁵ available at a resolution of 0.125 by 0.0625 degrees, and were speciated into the CB6 chemical mechanism species considered in the CAMx simulation⁶.

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

² 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

³ 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

⁴ 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

⁵ 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

⁶ 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 Portuguese Informative Inventory Report⁷ and on the emission sources, the main sectors contributing to PM₁₀, PM_{2.5} and NO₂ 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 Aveiro Region urban area (the receptor area considered for source apportionment) through the PSAT application.

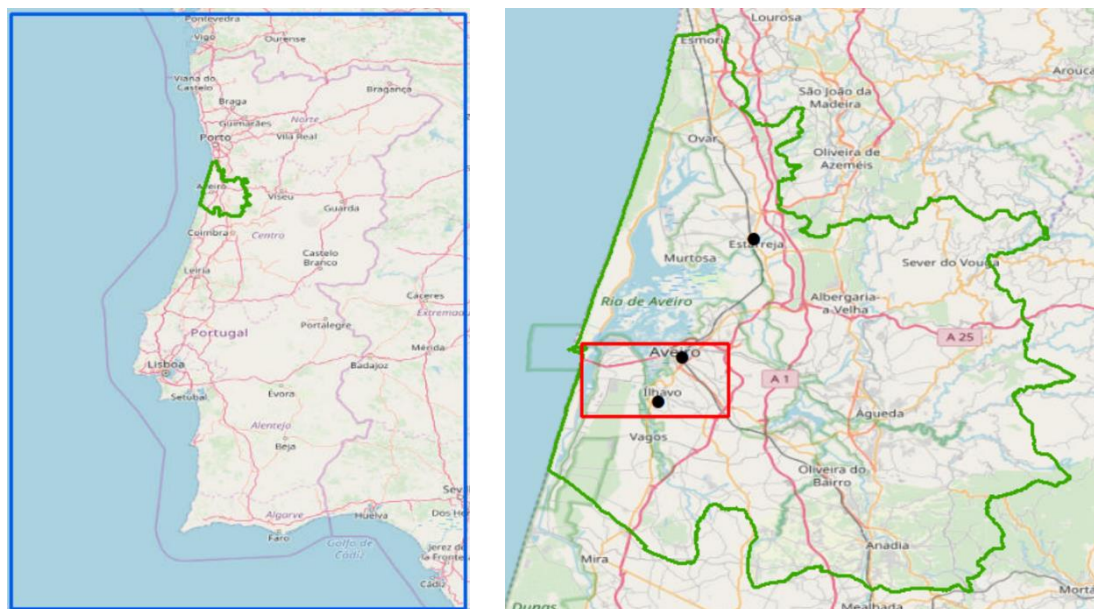


Figure 1 – (left) Blue square - CAMx nested domain with 0.05° horizontal resolution. Green contour – Aveiro Region area. (right) Green contour – Aveiro Region area. Black points – (from north to south) Estarreja, Aveiro and Ílhavo air quality monitoring stations, used to evaluate the model performance. 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 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

⁷ Pereira TC, Seabra T, Pina A, et al (2018) Portuguese Informative Inventory Report 1990-2016. Portuguese Environmental Agency

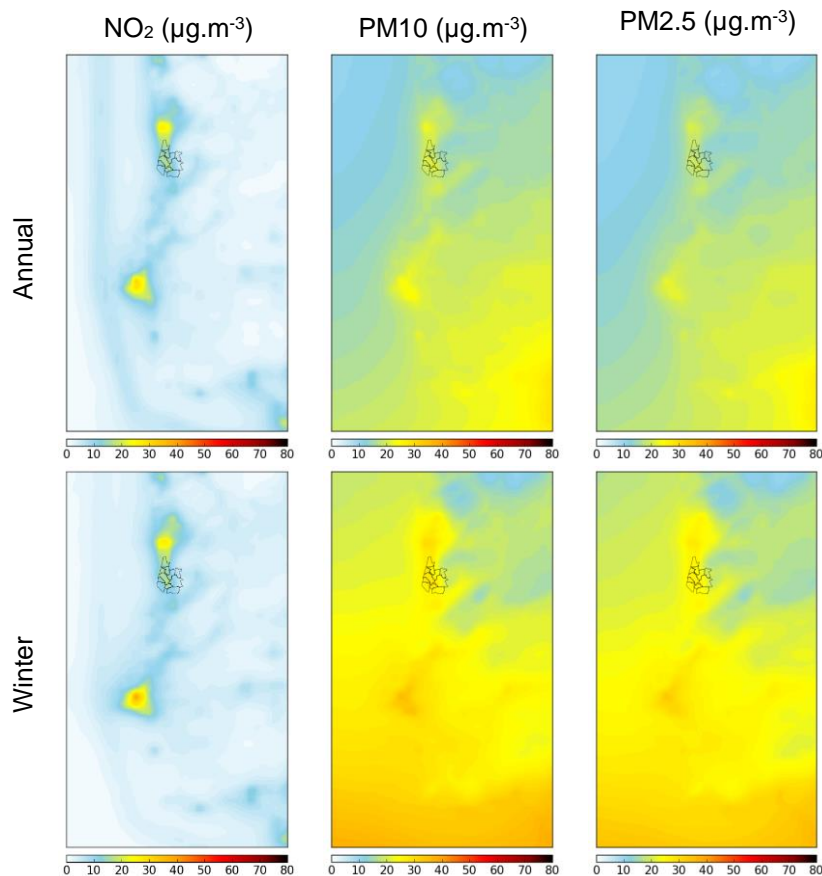
2. ANALYSIS OF RESULTS

2.1. Air quality assessment

The air quality characterization in the Aveiro 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 NO₂, PM10 and PM2.5 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 PM10, PM2.5 and NO₂ 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 PM10, PM2.5 and NO₂ concentration simulated for the urban area of Aveiro Region (URB) which was the receptor area defined in the PSAT application (see Fig. 2).

2.1.1. Concentration Fields

Fig. 2 presents the NO₂, PM10 and PM2.5 concentration fields obtained by the WRF-CAMx application for the three periods previously defined. For all pollutants, the results show similar spatial patterns for the different periods analysed. For PM10 and PM2.5 the concentration values shows a gradient decreasing from south to north. However, for NO₂, the highest concentration values are obtained in other urban areas within the domain, such as Porto (in the North) and Lisbon (in the Centre).



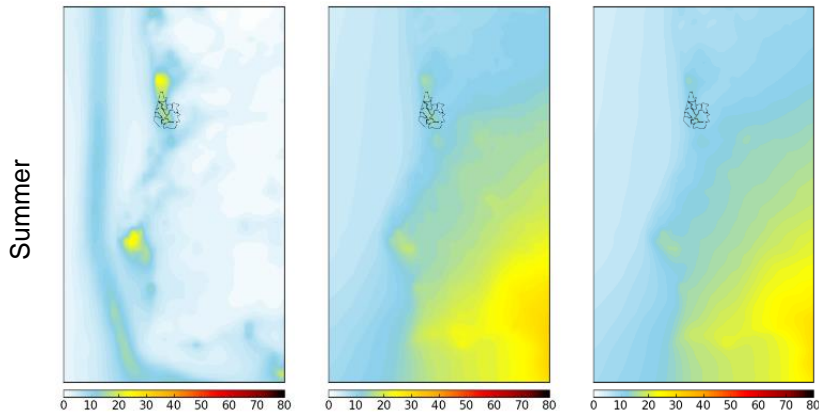


Figure 2 - Spatial distribution of NO₂, PM₁₀ and PM_{2.5} concentrations.

2.1.2. Source contribution analysis

The contribution of each source group for PM₁₀, PM_{2.5} and NO₂ 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 PM₁₀, PM_{2.5} and NO₂ concentrations, for the entire year of 2010.

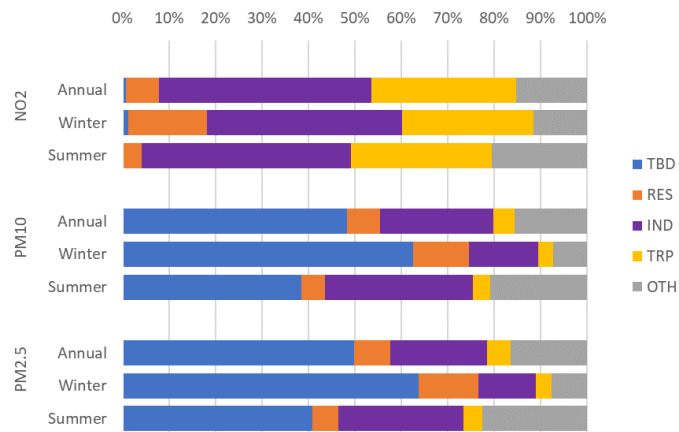


Figure 3 – Annual, winter and summer averages contribution for each source group for for PM₁₀, PM_{2.5} and NO₂ concentrations.

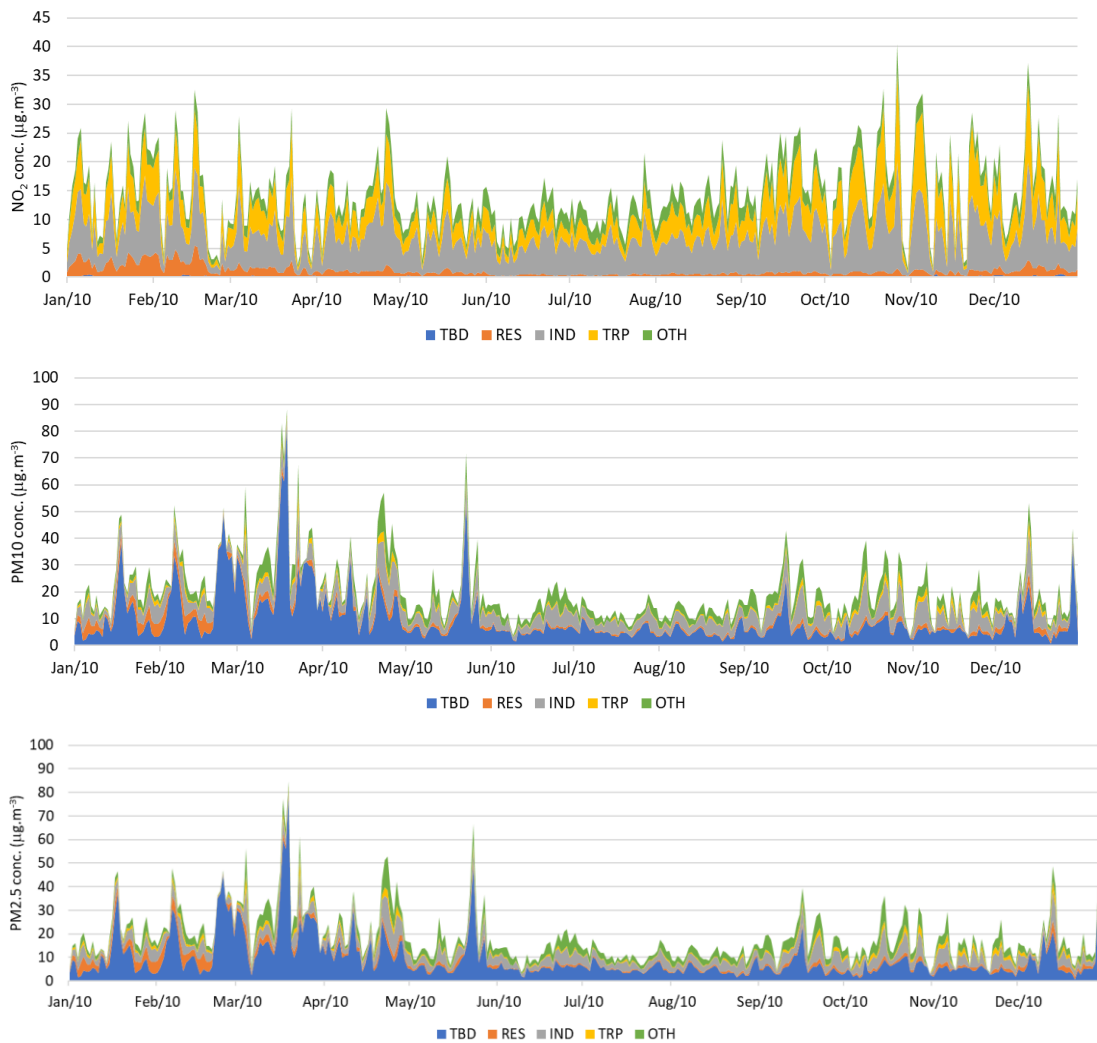


Figure 4 – Time series of daily average contributions for each source group for NO₂, PM₁₀ and PM_{2.5} concentrations.

For NO₂, the annual average contributions of each source group reveal that the major contribution is from industrial combustion and processes, with values up to 45%, followed by road transport, with 30%. In winter, residential and commercial combustion has a relevant contribution, close to 20%, while in summer its contribution is quite small. The annual average contributions of each source group reveal that one of the major contribution is from TBD (48%), highlighting the importance of transboundary transport for the PM pollution in the study region, especially from dust from the Sahara desert. This background/transboundary effect is even more notorious in the winter period, with values above 60%. Source contribution results also point to a great influence of the contribution of different human activities, such as industrial combustion and processes and residential combustion, to the PM levels.

Although the other sources (OTH) have a significant contribution for NO₂, PM₁₀ and PM_{2.5} 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 Estarreja, Aveiro and Ílhavo 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 Estarreja, Aveiro and Ílhavo air quality monitoring stations, considering the observed data as reference.

Air quality station	Pollutants measured	Station efficiency (%)	FB (-)	RMSE ($\mu\text{g}\cdot\text{m}^{-3}$)	r (-)
Aveiro	NO ₂	82.78	-0.57	23.06	0.28
Estarreja	NO ₂	98.32	-0.25	17.65	0.40
Ílhavo	NO ₂	71.32	0.18	10.18	0.58
Ílhavo	PM10	85.14	-0.29	19.40	0.22

In average, the RMSE, the standard deviation of the differences between the modelled and the observed values, is below 23 $\mu\text{g}\cdot\text{m}^{-3}$, and the correlation between modelled and observed values are between 22% and 58%. For FB, negative values are obtained, except for NO₂ in Ílhavo air quality monitoring station, showing an underestimation of the model results, compared with the observed values.