

CALIOPE-URBAN: COUPLING R-LINE WITH CMAQ FOR URBAN AIR QUALITY FORECASTS OVER BARCELONA

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1. INTRODUCTION

Barcelona is located in the north east of the Iberian Peninsula, is surrounded by the Mediterranean sea, two rivers and a mountain range. Barcelona has a very high vehicle density (approx. 5500 vehicles/km²) being the majority diesel (64%). Traffic stations in the city report chronic nitrogen dioxide (NO₂) exceedances of the European annual limit since the year 2000 and a 68% of citizens were exposed in 2016 to NO₂ levels above the annual limit (ASPB, 2017). European regulations recommend that an air quality forecasting system should be used by the administrations to inform public and decision makers about air quality levels, especially during air quality episodes.

In urban environments NO₂ present strong concentration gradients near roadways that cannot be reproduced by mesoscale air quality models since large concentration variations can occur within a grid cell (Pay et al., 2014). In order to overcome this limitation, the combination of regional and urban scale models is presented as a solution to estimate air quality at the street level within the larger grid cell.

This work describes a methodology to couple CALIOPE (Pay et al., 2012), a mesoscale air quality modelling system that provides 48 hour air quality forecasts at 1 km over Barcelona city, with the Research LINE source dispersion model (R-LINE). R-LINE (Snyder et al., 2013) was developed to predict strong gradients for roadways, which has been adapted to provide air quality estimates at street level within Barcelona's geometrical morphology (i.e. street canyon pattern).

The coupled modeling system is evaluated using street-level pollutant concentrations and meteorological measurements collected during a field study in April 2013 conducted by IDAEA-CSIC and compared with the current mesoscale solution applied to Barcelona.

2. METHODOLOGY

2.1 CALIOPE air quality system

The CALIOPE system integrates the Weather Research and Forecasting meteorological model (WRF), the High-Resolution Modelling Emission System (HERMES; Baldasano et al., 2008), the Community Multiscale Air Quality Modeling System (CMAQ) and the mineral Dust REgional Atmospheric Model (BSC-DREAM8b). The mesoscale system is run over Europe at a 12 km × 12 km horizontal resolution, Iberian Peninsula at 4 km × 4 km, and the Barcelona domain at 1 km × 1 km. CMAQ vertical levels are collapsed from the 38 WRF levels to 15 layers up to 50 hPa with six layers falling within the PBL. CMAQ version 5.0.1 with CB05 chemical mechanism and AERO5 aerosol scheme is used.

2.2 CALIOPE-Urban

The combination between CALIOPE and R-LINE, CALIOPE-Urban, requires the use of CMAQ for background concentration data and WRF for meteorological inputs. WRF bottom layer over the street of interest is used as boundary conditions for R-LINE local meteorology module. With respect to background concentrations, the upwind urban background scheme is applied. The upwind background scheme chooses CMAQ grid cell values depending on wind speed and direction. R-LINE local meteorology and upwind urban background scheme are implemented as part of the CALIOPE-Urban project. Additional

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results of these works will be presented in *Adaptation of meteorology and R-LINE to street canyon micro-climates: Application in Barcelona city (Spain)* by Michelle Snyder and *Influence of NO₂ - O₃ urban background on nitrogen dioxide concentration near roadway sources in Barcelona city (Spain)* by Jaime Benavides at 4:45 pm on Tuesday 10/24/2017.

To produce R-LINE hourly emissions inputs for each road segment, we compute hourly emissions using HERMES average annual emissions for each segment and HERMES temporal profiles.

R-LINE is run using the numerical integration approach to solve Gaussian dispersion equations and the Generic Reaction Set (GRS) for NO-NO₂-O₃ chemical reactions (Valencia et al., Submitted). Receptors are located forming a regular grid of 10 meters (m) horizontal resolution to predict spatial patterns and in specific coordinates to compare with observations.

2.3 Observations

To evaluate predicted hourly NO₂ we use observations from the official XVPCA network and from an experimental campaign conducted in April 2013 in Barcelona (Amato et al., 2014). In this work, we focus on the period 4-9 April to visually analyse temporal variation because it represents the main NO₂ concentration patterns found during this month. A longer period, which includes a one week air pollution episode, is used to statistically evaluate model performance (3rd to 24th April). During the campaign, mobile laboratories placed at the parking lane of several street segments measured air quality parameters at 3 m height. For this study, data gathered every 30 minutes at Industria Street No. 213, Industria Street No. 309 and Valencia Street No. 445 are used. These streets present a marked canyon pattern where building height to street width ratio is approximately 1.

3. RESULTS

To compare hourly NO₂ temporal variation in Barcelona streets between CALIOPE-Urban and CALIOPE we use observations from three sites with different conditions regarding emissions and geometry. First, an urban background site from the official network, Palau Reial, which NO₂ mean hourly concentration level during the whole period of study (3rd to 24th April 2013) was 40.7 µg/m³, while the average daily traffic on the closest street

for the year 2009 was 3900 vehicles. Palau Reial site is located in an open area at a distance of 220 m from a highly trafficked street. Second, a traffic monitoring site from the official network, Gracia. This site had a mean NO₂ level during the study period of 59.8 µg/m³, it is close to two streets with an average daily traffic of 15600 vehicles and it is located in a square, surrounded by buildings of 5-6 stories tall. This site is heavily influenced by NO₂ urban background because its mean annual levels are among the highest in the city, while it has less traffic than other monitoring sites. The high NO₂ concentrations are due to Barcelona's high vehicle density (i.e. 5500 vehicles/km²) being the majority diesel. Third, Valencia Street No. 455 site from the experimental campaign that is located in a highly trafficked street with a mean hourly NO₂ during the period of study of 70.1 µg/m³ and an average daily traffic of 32500 vehicles. Valencia Street represents the typical street canyon pattern with 20 m building height and 20 m street width.

3.2 Model performance analysis

Figure 1 shows the temporal variation of NO₂ hourly concentration levels during the initial 4 day period of the study (Thursday 4th to Monday 8th of April 2013) in Palau Reial. The mesoscale system (blue line) represents remarkably well the main pattern found in the observations but it does not reproduce the peak observed on 8th April morning. The street scale system, CALIOPE-Urban, does not provide an overall improvement on this site due to the restricted influence of local traffic sources.

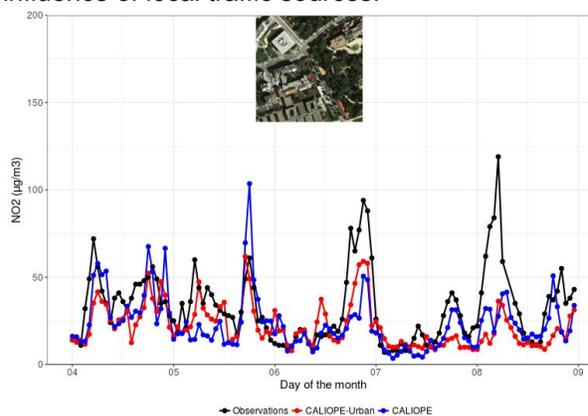


Figure 1. NO₂ hourly variation for the period 4th to 8th April 2013 in Palau Reial station. Observations represented in BLACK, CALIOPE-Urban in RED, and CALIOPE in BLUE. The top image is the site viewed from above.

Next in Figure 2, hourly NO₂ concentrations from 4th to 8th of April in Gracia station are compared. The mesoscale solution reproduces observation behaviour but tends to underestimate afternoon levels. In contrast, the street scale system increases afternoon levels and gives a better estimate of concentration peaks.

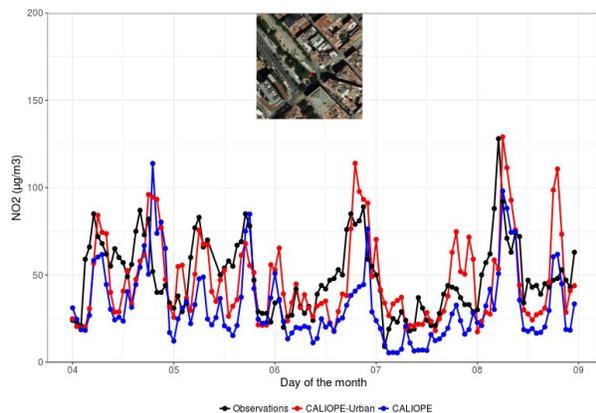


Figure 2. NO₂ hourly variation for the period 4th to 8th April 2013 in Gracia. Observations shown in BLACK, street-scale model in RED, and mesoscale in BLUE. The top image is the site observed from above.

Finally, Figure 3 shows NO₂ levels for the same period (4th to 8th April 2013) in the highly trafficked experimental site of Valencia Street No. 455. From Figure 3 we can see a higher difference in performance between mesoscale and street-scale models. Overall mesoscale is systematically underpredicting the concentration during the central hours of the day and is not able to capture the peaks. In contrast, street-scale represents more precisely the measured diurnal variation, giving estimates on weekdays in accordance with observations levels and a better reproduction of peak values. For example, on the 8th at 6 am (UTC) a concentration peak found in observations (136.5 µg/m³) is better reproduced by street-scale (128.7 µg/m³) than by mesoscale (72.4 µg/m³). It is also remarkable the improvement of CALIOPE-Urban during the central hours of the day.

We argue that difference of model performance from Figures 1, 2 and 3 is directly related to the broad spectrum of urban geometry and traffic conditions found in Barcelona city. In Figure 3, is shown that to reproduce NO₂ levels in streets with high traffic intensity is necessary to

resolve local processes such as near road sources dispersion and chemistry.

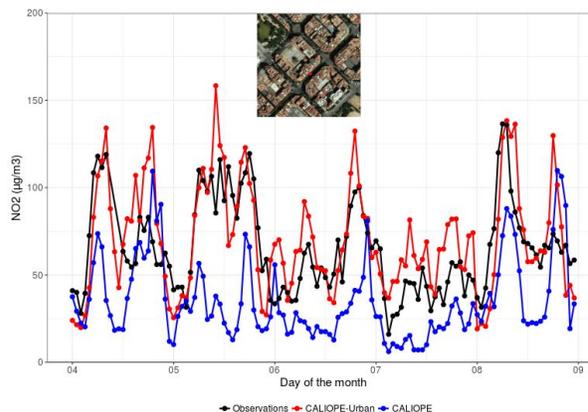


Figure 3. NO₂ temporal variation for the period 4th to 8th April 2013 in Carrer Valencia No. 455. Observations shown in BLACK, street-scale model in RED, and mesoscale in BLUE. The top image is the site seen from above.

The predicted hourly NO₂ levels have been compared with observations for the entire period of study (3rd to 24th April 2013) in the sites analysed above. Table 1 shows the performance statistics highlighting the better performance of street-scale in intense traffic sites.

		FAC2	MB	RMSE	r
	CALIOPE	0.70	-4.08	27.86	0.55
	CALIOPE-Urban	0.66	-8.26	27.72	0.47
	CALIOPE	0.58	-13.97	34.33	0.50
	CALIOPE-Urban	0.73	-3.36	33.85	0.42
	CALIOPE	0.55	-20.99	37.81	0.53
	CALIOPE-Urban	0.91	5.02	28.93	0.57

Table 1. Performance summary statistics for period 3rd to 24th April 2013. Top values refer to Palau Reial (Background), middle to Gracia (traffic) and bottom to Valencia Street No. 455 (traffic)

For instance, 91% of model results are within a factor of two of the observations in Valencia Street No. 455. Furthermore, there is a better correlation between its results and observed hourly NO₂ levels in Valencia Street No. 455 (r =

0.57) than mesoscale (0.53). However, in Gracia site the correlation is lower, which can be explained by the high NO₂ background contribution to this site. Mesoscale produces better results for the background site Palau Reial with small negative biases of 4.08 µg/m³ compared to its performance in traffic sites where it gives a higher negative bias (e.g. Valencia Street No. 455 20.99 µg/m³).

The RMSE shows model results closer to observations in street-scale for traffic sites and slightly better for mesoscale in the background site.

Figure 4 shows the spatial detail provided by street-scale and mesoscale combined solutions over Eixample district for an hour randomly chosen from the study period. The increased resolution of street-scale makes possible to visualize NO₂ street gradients.

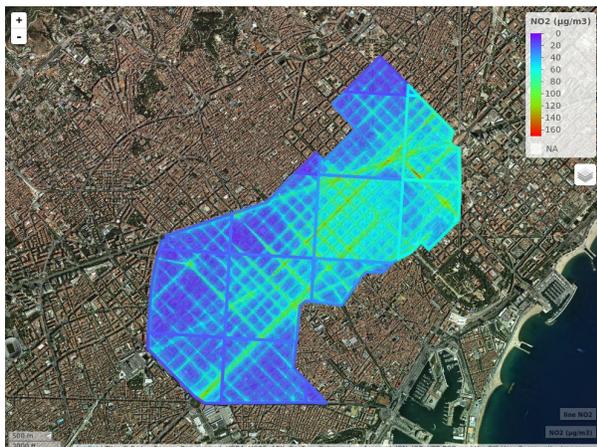


Figure 4. NO₂ hourly level at 8 am (UTC) on 9th April 2013. Squares represent mesoscale grid cell values and the inside content street-scale concentrations

4. CONCLUSION

In urban environments NO₂ present strong concentration gradients at street level that cannot be reproduced by mesoscale air quality models. We coupled a mesoscale air quality model, CALIOPE, with a dispersion model, R-LINE. R-LINE has been adapted to estimate NO₂ hourly levels under Barcelona geometrical conditions by considering specific meteorological conditions for each street.

The developed system, CALIOPE-Urban, has been evaluated in comparison with the mesoscale system and observations in three sites with different conditions of geometry and emissions. The street-scale model gives better results than

the mesoscale near trafficked areas where is able to reproduce morning and evening concentration peaks. However, CALIOPE-Urban does not reproduce precisely NO₂ patterns in traffic sites that are highly influenced by urban background. Hence, a subsequent effort to better represent urban background concentrations is necessary.

With its current configuration, CALIOPE-Urban reproduces large concentration variations that exist within a mesoscale system grid cell.

Disclaimer

The results presented here are part of ongoing research and should not be used or referenced until the research is complete and published. If you wish to use results from this extended abstract please contact the corresponding author (Jaime Benavides: jaime.benavides@bsc.es)

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