EVALUATING THE IMPACT OF INCREASING HORIZONTAL RESOLUTION ON AIR QUALIY MODELLING SYSTEMS OVER BIG METROPOLITAN AREAS IN SPAIN

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1. INTRODUCTION

The definition of the grid resolution is an important decision when applying an air quality modeling system. The horizontal grid size should be able to reproduce the atmospheric circulations of the modeling area determined by the topography, i.e. the complexity of the Iberian Peninsula forces to utilize resolutions ranging from 1 to 5 km (Jiménez et al., 2005). But, even with the finest scale, the modeled concentrations are not necessary the better (Valari and Menut, 2008). This paradoxical result is mainly due to the fact that by increasing emissions and meteorology spatial resolution, uncertainties also increase with the risk of model error. Even more, computational cost increases markedly with the inverse of the grid spacing, which could be important in terms of computational resources to air quality forecast. However, the advancement of performance computing allows to increase model resolution and to investigate multiple spatial scales with the aim to establish the adequate grid size to forecast air quality at local scales.

Several studies have evaluated the impact of increasing horizontal resolution on O_3 on different scales and particulate matter and its components. Recently, the co-operative programme for monitoring and evaluation of the long-range transmission of air pollutants in Europe (EMEP) in collaboration with five European modeling teams have been performed a study to determine the effect of grid resolution in air quality modeling performance over the European domain at regional and urban scale (Cuvelier et al., 2013). A model inter-comparison exercise with five chemical transport models (EMEP, CHIMERE, CMAQ, LOTOS-EUROS and RCGC) as a function of four resolutions (56 km x 56 km, 28 km x 28 km, 14 km x 14 km, and 7 km x 7 km), showed that it is difficult to define a grid size that is adequate to resolve the urban signal under all conditions affecting Europe, but 14 km resolution seems to be a good compromise between a pure background application and an application which reproduces most of the urban signals (7 km resolution).

In Europe, operational air quality systems use resolution between 12-25 km, meanwhile application to a single country can reach resolution between 4-10 km (Zhang et al., 2013). In the Spanish context, the Barcelona Supercomputing Center-Centro Nacional de Supercomputación (BSC-CNS) predicts air pollution with high spatial resolution over Spain (4 km x 4 km) by means the CALIOPE Air Quality Forecast System (CALIOPE-AQFS; Baldasano et al., 2011; Pay et al., 2012). Data assimilation techniques and evaluation in near real time are performed in order to provide accurate air quality forecasts.

Thanks to the high performance computing resources at the BSC-CNS, the present work aims to assess the impact of increasing horizontal resolution from 4 km to 1 km over Barcelona and Madrid metropolitan areas (BCN and MAD) together with the Andalusia region (AND), which represent the most populated areas affected by different emission patterns and atmospheric dynamics. For that purpose, CALIOPE-AQFS forecasts air quality at two horizontal resolutions, a first domain covering Spain at 4 km (IP4), and a second domain over Andalusia region (AND1), Barcelona (BCN1) and Madrid (MAD1) at 1 km. The study is performed over April 2013 based on the main pollutants O_3, NO_2, SO_2, and PM10.

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2. METHODOLOGY

2.1 CALIOPE-AQFS

The CALIOPE-AQFS, composed by a set of models: WRF-ARWv3.2.1 meteorological model, the High-Elective Resolution Modelling Emission System (HERMESv2), a mineral dust dynamic model (BSC-DREAM8bv2), and the CMAQv5.0.1 chemical transport model, provides air quality forecast for 48h over Spain at 4 km x 4 km (www.bsc.es/caliope). First, CALIOPE is run over Europe (the mother domain) at 12 km x 12 km using the pollutant concentration from the global model LMDz-INCA to feed the boundary conditions. Then, CALIOPE is run at higher resolution over the Iberian Peninsula at 4 km x 4 km (IP4) using a one-way nesting. In the present work CALIOPE AQFS is run at 1 km x 1 km over the domains at hands (AND, BCN and MAD) by means a nesting over IP4, namely AND1, BCN1 and MAD1, respectively.

HERMESv2 estimates emissions over Europe following a top-down disaggregation from the EMEP inventory. Over the Spanish domain, the HERMESv2 model (Guevara et al., 2013) forecasts anthropogenic and biogenic emissions at 1 km x 1 km and 1 h following a bottom-up methodology. For AND1, BCN1 and MAD1 simulations emissions remain at 1 km x 1 km, meanwhile for IP4, emissions are aggregated into 4 km x 4 km grids.

2.2 Study area

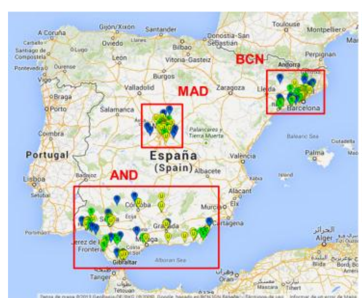
The work is focused over Barcelona and Madrid metropolitan areas (BCN and MAD) together with the Andalusia region (AND) (Figure 1), which represent the most populated areas in Spain with very complex terrains and affecting by different emission patterns. BCN and MAD are the most populated cities of Spain. BCN It is a coastal area characterized by a very complex terrain (several valleys perpendicular to the coastal line, two mountain ranges: coastal (500 m) and pre-coastal (1000-1700 m)) which induces a dynamic dominated by mesoscale phenomena such as sea-breeze recirculation and mountain-valley. On the other hand, MAD is a continental region with a much simpler topography (Central System located in the north-western area of the domain, with summits reaching 2500 m, and the Tajo valley in the southern area), which brings different locally-driven flows.

In BCN the urban contribution (3.1 million inhabitants) is accompanied by industrial and power generation emissions, the road network and the harbor, meanwhile in MAD, the Spanish capital, is mainly under the influence of emission from the urban area (5.8 million inhabitants) and the road network that connects MAD with surrounding industrial and urban areas.

AND is the southern-most region in Spain with a complex topography characterized by the large depression of the Guadalquivir Basin (delimited by the Iberian Massif and the Betic Range), that crosses the region from NE to SW along 60 km. About three quarters of AND has a mountainous orography, including Sierra Nevada (3481 m). AND includes a big city (Seville, > 400.000 inhabitants), others medium cities (e.g. Huelva) and important industrial areas devoted to industrial processes, electric generation and maritime traffic such as Strait of Gibraltar.

2.3 Evaluation method

The comparison between both CALIOPE-AQFS grid resolutions is done in terms of gas-phase and aerosol concentrations (O_3, NO_2, SO_2 and PM10) at the lowest level. Modeled concentrations are compared against observations on an hourly basis. A number of 80 monitoring stations provide measurements to evaluate AND, 46 for BCN, and 45 for MAD. Figure 1 shows the location of the air quality stations over the domains at hand, and the number of sites for each pollutant. The evaluation is based on classical statistics such as correlation coefficient (r), Mean Bias (MB), and Root Mean Square Error (RMSE) performed on an hourly basis. The influence of the type of station is taken into account according to different categories: rural stations (R), suburban stations (S), urban stations (U). The study is performed over April 2013.



	AND		BCN		MAD		Total	
	80		46		45		171	
Pollutant								
O_3	49		30		36		115	
NO_2	73		34		45		152	
SO_2	63		31		19		113	
PM10	54		15		33		102	
Area		%		%				%
Urb	37	46	21	46	32	71	90	53
Subur	28	35	18	39	7	16	53	31
Rur	15	19	7	15	6	13	28	16

Fig. 1. Domains of study: Andalusia (AND), Barcelona (BCN), and Madrid (MAD); and characteristics of air quality stations available for April 2013.

3. RESULTS

3.1 Monthly evaluation

Table 1 summaries the monthly statistics (r and RMSE) computed at 4 km (IP4) and 1 km (AND1, BCN1 and MAD1) for O_3, NO_2, SO_2, and PM10 in each domain (AND, BCN and MAD). The impact of increasing resolution depends on lifetime of the studied pollutant, as well as their variability and dependency with their precursor concentrations. O_3 is the pollutant which presents a low impact with resolution increase, where correlation coefficients show a low variability (less than 4 %). For the primary pollutant NO_2, the correlation coefficients increase ~ 3-4%, except for BCN. The resolution change has the highest impact on SO_2 model performance, increasing correlation coefficient ~ 10-17% in the urban domains of MAD and BCN, but increasing errors in BCN and AND (~2-3µgm^{-3}). In contrast, the resolution increase has the lowest effect in PM10 model performance, showing a lightly increase of RMSE around 1-2 % in both domains (<1µgm^{-3}) over the three domains.

Table 1. Monthly mean correlation coefficient (r) and root mean square error (RMSE, µgm^{-3}) for the three domains (Andalusia, AND; Barcelona, BCN; and Madrid, MAD) over April 2013 as a function of resolution (1 km and 4 km).

	Study	R		RMSE	
	domain	1 km	4 km	1 km	4 km
O_3	AND	0.53	0.55	25.5	25.3
	BCN	0.50	0.50	29.0	27.6
	MAD	0.65	0.66	21.9	22.4
NO_2	AND	0.26	0.25	10.9	10.5
	BCN	0.35	0.35	24.6	24.2
	MAD	0.61	0.59	15.3	15.7
SO_2	AND	0.14	0.14	9.8	8.1
	BCN	0.11	0.10	8.8	5.7
	MAD	0.21	0.18	3.4	3.5
PM10	AND	0.53	0.52	17.7	17.5
	BCN	0.36	0.37	17.1	16.8
	MAD	0.50	0.50	14.7	14.3

Due to differences in topography and emission pattern over the three domains at hands, the resolution increase has different impacts. MAD is the city where the resolution increase has the greatest effect. Madrid is mainly affected by traffic emissions, so an accurate allocation of primary emission has a positive impact increasing r and reducing RMSE for NO_2 and SO_2. Over all the stations, NO_2 correlation coefficient increases from 0.59 (4 km) to 0.61 (1 km), and 0.18 (4 km) to 0.21 (1 km) for SO_2. For both pollutants, RMSE decrease a 3% when resolution increases. However, for O_3 the error increases by 2% (~0.5µgm^{-3}) and r decreases from 0.65 to 0.66 when resolution increases. In BCN the increase of resolution does not significantly improve temporal correlation for all the pollutants, but errors increase ~ 2-5%, except for SO_2. This low effect of resolution increase on temporal statistics is shown in AND, where errors increase from 8 to10 µgm^{-3}. SO_2 is the pollutant showing the lowest performance at both resolutions, with large bias and very low r on an hourly basis. The reason for such a low performance at 1 km is understudy.

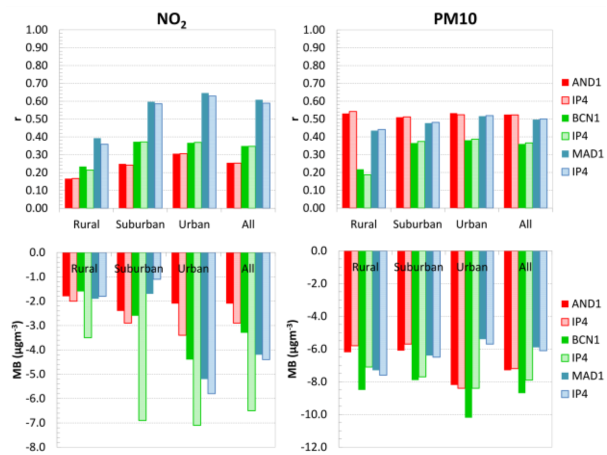


Fig. 2. Bar plot for monthly r and MB by station type for NO_2 and PM10. Colors indicate the domain (red, AND; green, BCN; and blue, MAD). Dark color bars indicate simulation at 1 km resolution, and light color bars indicate simulation at 4 km resolution.

The resolution impact also depends on the environment and direct emission directly affecting air quality. Figure 2 shows a bar plot diagram for r and RMSE as function of station type and study domain for NO_2 and PM10. For NO_2, the resolution increase does not significantly change correlation coefficient as a function of station type, only the urban stations of MAD depict an improvement from 0.63 (4 km) to 0.65 (1 km). However, NO_2 biases decrease when resolution increase from 4 km to 1 km at urban station around 38 % for AND and BCN, and 10% in MAD. For PM10, the impact of resolution increase is quite low for correlation coefficient (~2%, except for urban stations in BCN).

3.2 Spatial pattern

The monthly spatial variation of increasing resolution for NO_2 concentration is further analyzed in Figure 3 for the three domains. Overall, the explained spatial variability improves as function of resolution for all the pollutants support by the increase of the monthly r, from 0.82 (4 km) to 0.84 (1 km) for NO_2. The slopes significantly improves with resolution increase from 0.70 (4 km) to 0.75 (1 km), dominated by the improvement of model behavior in urban stations, indicating that CALIOPE-AQFS explain better the magnitude of the variability between urban regions at 1 km. Although not shown here, the spatial correlation coefficient increase for the other primary pollutant SO_2, from 0.39 (4 km) to 0.46 (1 km); and slightly decrease for the secondary pollutant, from 0.61 (4 km) to 0.53 (1 km) for O_3, and 0.53 (4 km) to 0.50 (1 km) for PM10.

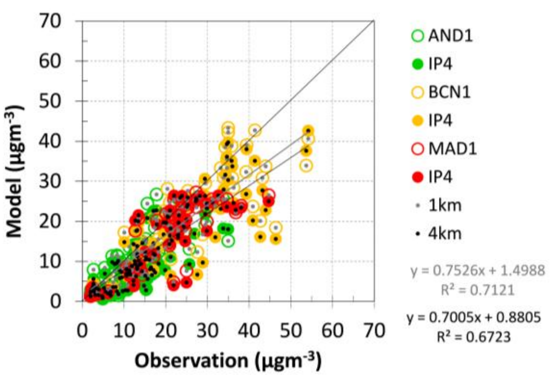


Fig. 3. Monthly NO_2 mean modeled concentrations versus observations for each study domain as function of horizontal resolution. Equations show the linear adjusts between model and observation at 1 km (light grey) and 4 km (dark grey).

To analyze the impact of increasing horizontal resolution on the pollutant dispersion, Figure 4 shows the monthly mean NO_2 concentration during April 2013 over MAD domain at 4 km x 4 km (top) and 1 km x 1 km (bottom), respectively. The dots show mean concentrations at air quality stations, and they help to evaluate the spatial representativeness of the NO_2 simulated at different resolutions. In MAD on-road traffic constitutes the main source of primary pollutants in the region; 75% of NO_x emissions are produced by on-road traffic, which constitutes the main source of primary pollutants in the region in MAD. The distribution of the urban plume follows the same direction (south-west to north-east) at both resolutions. However, the demarcation of main highways connecting the capital with the rest of the country is better shaped at 1 km than at 4 km. Note the high agreement between air quality stations and NO_2 concentrations near main suburban traffic roads.

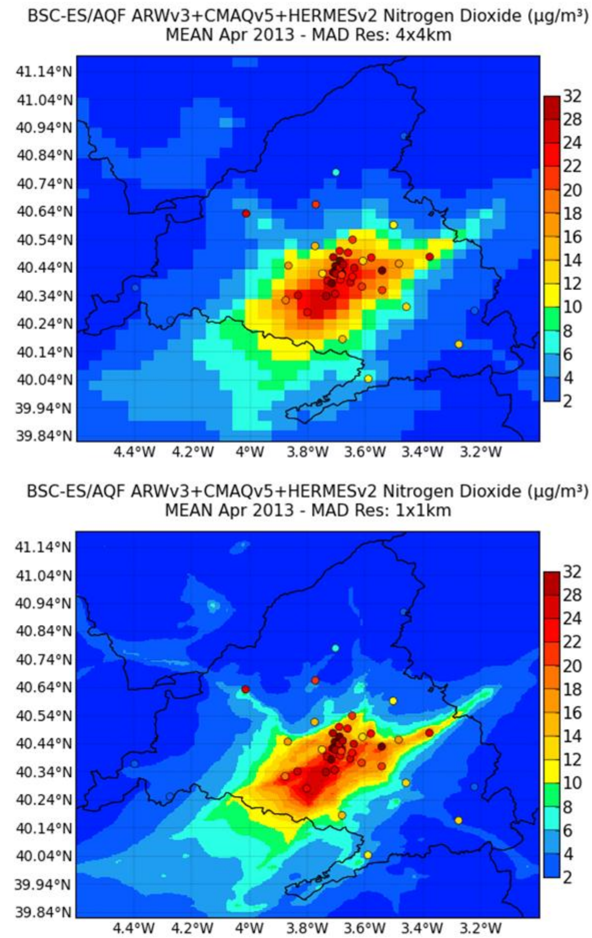


Fig. 4. Mean NO_2 modeled concentration over MAD for April 2013 at 4 km (top, IP4) and 1 km (bottom, MAD1) resolution. Dots indicate mean concentration at air quality stations.

As in MAD, on-road traffic constitutes the main source of primary pollutants in BCN with a 57% of NO_x emitted by on-road traffic sector. Figure 5 depicts NO_2 concentration maps for 18 UTC 16th April 2013 at 4 km x 4 km (top) and 1 km x 1 km (bottom), respectively. Overall, the definition of traffic roads significantly increases from 4 km to 1 km, especially for those roads connecting the Barcelona city center with small cities around and industrial areas such as Tarragona in the southwestern part of the BCN domain.

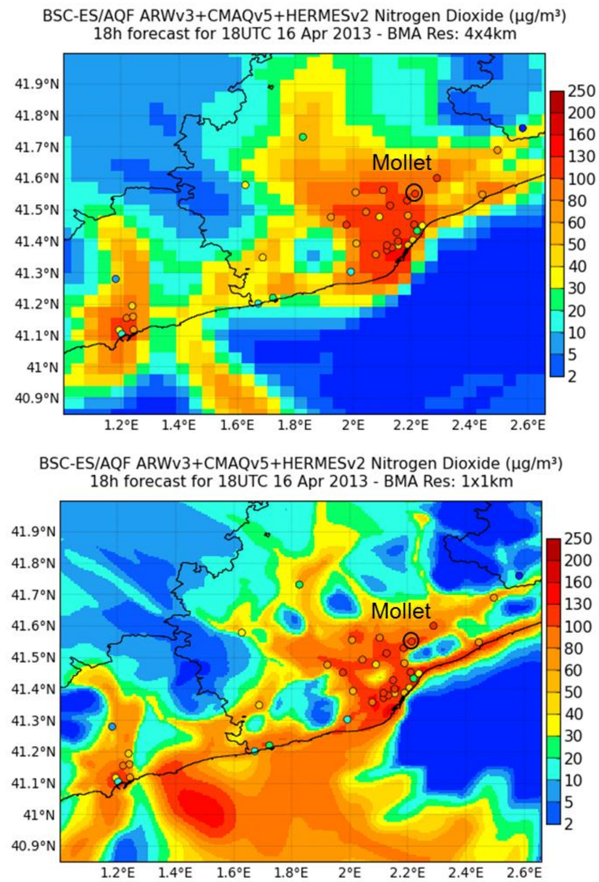


Fig. 5. Mean hourly NO_2 concentration over BCN for 18UTC 16 April 2013 at 4 km (top, IP4) and 1 km (bottom, BCN1) resolution. Dots indicate mean concentration at air quality stations.

Furthermore, the 1 km resolution simulation allows to reproduce realistic NO_2 concentration patterns according to the topography of the domain at hand. Note how at 1 km resolution, the NO_2 concentration along the coastal chain (500 m height) and pre-coastal chain (1000-1700 m) display the lowest concentration (< 10 µgm^{-3}), except for the city center urban hill where concentration reach 20-40 µgm^{-3}. In contrast, at 4 km resolution the NO_2 concentration over these complex terrains is smoothed with the concentration around and no decreasing concentration is detected.

Furthermore, the resolution increase shows how the calculated concentrations increase in Barcelona downtown and the harbor from 100-130 µgm^{-3} (4 km) to 130-160 µgm^{-3} (1 km), allowing to better allocate the peaks than at lower resolution.

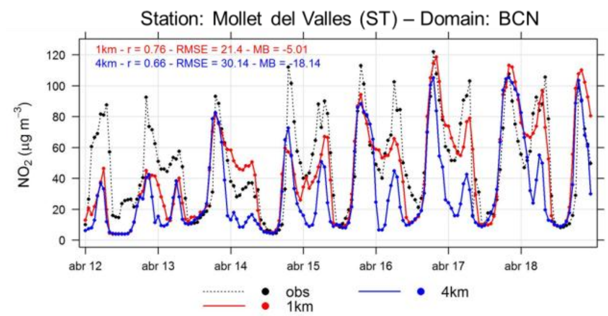


Fig. 6. NO_2 temporal series from 12nd to 18th April 2013 at Mollet station simulated by CALIOPE-AQFS at 4 km (blue lines) and 1 km (red lines) horizontal resolution. Black lines indicate observations. Statistics RMSE and MB (in µgm^{-3}) are shown in the top.

As shown in Figure 5, NO_2 concentrations at stations located near main suburban traffic roads display a higher agreement at 1 km resolution than at 4 km. For example, Figures 6 shows modeled and measured NO_2 temporal series at the Mollet stations in BCN domain (see Fig. 5). Hourly concentrations depict a remarkable daily cycle, since Mollet is a traffic stations located close to a highway connecting the Barcelona city. CALIOPE-AQFS NO_2 hourly concentrations improve when resolution increases. MB is reduced from -18 µgm^{-3} (4 km) to -5 µgm^{-3} (1 km) and temporal correlation increase from 0.66 (4 km) to 0.76 (1 km). CALIOPE-AQFS at 1 km reproduces better the early NO_2 peaks than 4 km, driven for the higher concentration during the last hours of the night and early morning.

4. CONCLUSION

The present work shows the effect of increasing the horizontal resolution from 4 km to 1 km in the CALIOPE air quality forecasting over the three study domains (AND, BCN and MAD) in terms of air quality concentrations.

The results indicate that the horizontal grid influence highly depends on the environment (from urban to rural), the studied pollutant and the study domain. Overall, the increase of the resolution, from 4 km to 1 km, improves the CALIOPE performance at stations near large emission sources.

The NO_2 shows an improvement with the resolution increases based on monthly correlation coefficient increasing ~ 3-4% (except of BCN), displaying the maximum increment at the urban stations of MAD from 0.63 (4 km) to 0.65 (1 km). Furthermore, the mean biases slightly decrease by ~1-3 µg m^{-3} in urban areas in AND, BCN and

MAD. The increase of grid resolution is not favorable for O_3 and PM10 especially at rural stations. For O_3, spatial r decreases from 0.61 (4 km) to 0.59 (1 km) in BCN rural stations since O_3 is secondary formed downwind from VOC and NO_x sources. Overall, the grid effect is less pronounced for PM10 than for O_3, because there is a part of the urban PM10 mass consists of secondary aerosols and this part is less affected by a decreasing grid size in contrast to the locally emitted primary components.

Although differences between both resolutions in terms of temporal monthly statistical is relatively low (MB and RMSE less than 3 µg m^{-3}, and r less than 0.1) the analysis of the concentration maps revels that NO_2 concentrations are better allocate at 1 km than at 4 km, and displaying a more realistic pattern, especially over the study complex terrains where NO_2 spatial correlation increase from 0.82 (4 km) to 0.84 (1 km). Furthermore, the increase of resolution allows to better capture the NO_2 daily cycles.

Based on the present results, the CALIOPE-AQFS provides forecast at 1 km x 1 km for Andalusia region, and Barcelona and Madrid metropolitan area using the HERMESv2.0 which provides accurate and realistic emissions in terms of the current Spanish emission patterns, based on the methodology improvements and updated to the reference year 2009.

5. ACKNOWLEDGMENTS

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