INFLUENCE OF HORIZONTAL GRID RESOLUTION ON AIR QUALITY MODELLING SYSTEMS IN BARCELONA METROPOLITAN AREA (SPAIN)

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Abstract: When applying an air quality model system, the definition of the horizontal grid resolution is an important point to take into account, especially over complex terrains as the Iberian Peninsula. The CALIOPE system forecasts air quality at high resolution for Spain (4 km x 4 km). The present contribution evaluates the impact of increasing the spatial resolution, from 4 km x 4 km to 1 km x 1 km, over the Barcelona Metropolitan Area in terms of the concentration of the main pollutants (O_3, NO_2, SO_2, and PM10). Modelled concentrations are compared against measurements from 49 monitoring stations (urban, suburban, and rural) from the Xarxa de Vigilància i Previsió de la Contaminació Atmosfèrica (XVPCA) providing near real time evaluation on an hourly basis. Despite the fact that differences between both resolutions in terms of annual statistics (September 1st 2011-September 1st 2012) is relatively low (MB and RMSE less than 3 µg m^{-3}, and r less than 0.1), the analysis of the concentration maps during a typical pollution episode revels that NO_2 concentrations are better allocate at 1 km than at 4 km, increasing the concentration (~20 µg m^{-3}) in Barcelona urban conglomeration and the harbour with high agreement with observations.

Keywords: *bottom-up, emissions, forecast.*

INTRODUCTION

The definition of the grid resolution is an important decision when applying an air quality modelling system. The results of the CityDelta project (Vautard et al., 2007) showed that 5 km horizontal resolution was enough to reproduce O_3 and PM10 over cities. However, the horizontal grid size should be able to reproduce the atmospheric circulations of the modelling 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 modelled 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.

In the Spanish context, the Barcelona Supercomputing Center-Centro Nacional de Supercomputación (BSC-CNS) has established the CALIOPE Air Quality Forecast System (CALIOPE-AQFS; Baldasano et al., 2011) to predict air pollution (O_3, NO_2, SO_2, and PM10) with high spatial resolution over Europe (12 km x 12 km) and the Iberian Peninsula (4 km x 4 km). A number of studies support the confidence on the system (Pay et al., 2012 and references therein). On the other hand, CALIOPE-AQFS is near real time (NRT) evaluated against air quality measurements on an hourly basis.

The Barcelona Metropolitan Area (BMA) is one of the largest Spanish urban areas where problems related to air quality and traffic derived emissions are of special concern. The present work aims to assess the grid horizontal resolution effect on model performance over the BMA. For that purpose CALIOPE-AQFS forecasts air quality at two horizontal resolutions, a first domain covering Spain at 4 km x 4 km, and a second domain over Barcelona and surroundings at 1 km x 1 km. The study is performed over a natural year from September 1st 2011 to September 1st 2012, in order to highlight the different behaviour of model performance and atmospheric dynamics in the target domain based on the main pollutants O_3, NO_2, SO_2, and PM10.

METHODOLOGY

The modelling system

The CALIOPE-AQFS, composed by a set of models: WRF-ARWv3.0.1.1 meteorological model, the High-Elective Resolution Modelling Emission System (HERMES04), a mineral dust dynamic model (BSC-DREAM8b), and the CMAQv4.5 chemical transport model, provides air quality forecast for 48h over Spain with high spatial and temporal resolution (4 km x 4 km, 1h) (www.bsc.es/caliope). Currently, CALIOPE AQF forecasts air quality across five domains at different horizontal resolutions: Europe (12 km x 12 km), Iberian Peninsula and Balearic Islands (4 km x 4 km), Andalucia and Canary Islands (2 km x 2 km); and BMA (1 km x 1 km). First, CALIOPE is run over Europe (the mother domain) using the pollutant concentration from the global model LMDz-INCA to feed the IBC. Then, CALIOPE is run at higher resolution over the smaller domains using a one-way nesting technique. For the present work we use two high horizontal resolution domains covering BMA, (1) the Spanish at 4 km x 4 km (IP4); and (2) the Barcelona domain at 1 km x 1 km (BCN1).

HERMES04 estimates emission over Europe following a top-down disaggregation from the EMEP inventory. Over the Spanish domain, the HERMES04 model (Baldasano et al., 2008) forecasts anthropogenic and biogenic emissions at 1 km x 1 km and 1 h based on the reference year 2004 following a bottom-up methodology. In the case of the BCN1 domain, emissions remains at 1 km x 1 km (Figure 1, right), meanwhile over IP4 domain, emissions are aggregated into 4 km x 4 km grids (Figure 1, left).

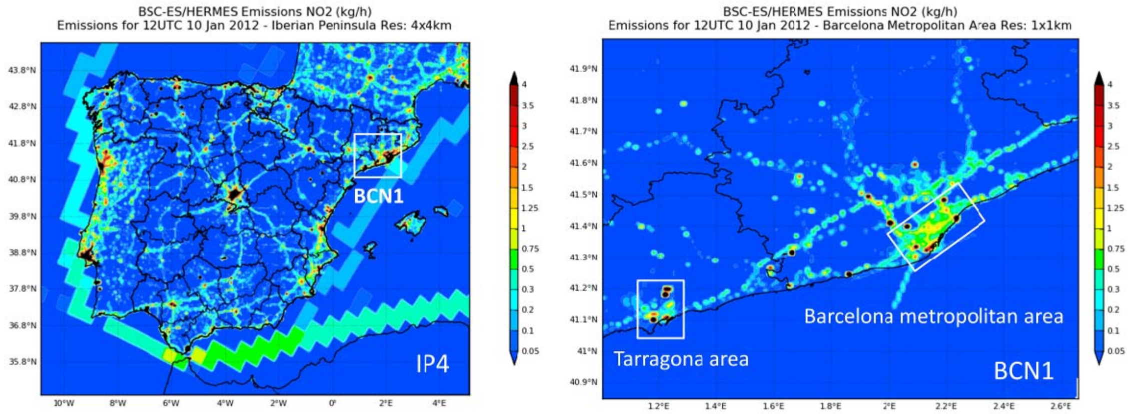

Figure 1. CALIOPE domains covering BMA: left at 4 km x 4 km (IP4); and right at 1 km x 1 km (BCN1). Colour chart shows NO_2 emission rate (kg/h) for January 10th 2012 at 12UTC.

The study area

The study is focused on the Barcelona Metropolitan Area (Figure 1), one of the most populated cities of Spain. 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 (Pérez et al., 2004). Figure 1 shows the NO_2 emission pattern over the study domain which includes both the BMA and the Tarragona area corresponding to January 10th 2012 at 12UTC. Inside the BMA, the urban contribution (3.1 million inhabitants) is accompanied by industrial and power generation emissions, the urban road network and the Barcelona harbour. Outside the BMA, a significant source of pollutants (NO_2, PM10 and SO_2) is Tarragona industrialized area. Although Tarragona is ~100 km far away from Barcelona, its industrial plumes influence the background levels of the BMA under some meteorological situation (and vice versa). The road network connecting the Mediterranean coast from Algeciras to France (AP-7 or E-15), is another significant source of NO_2.

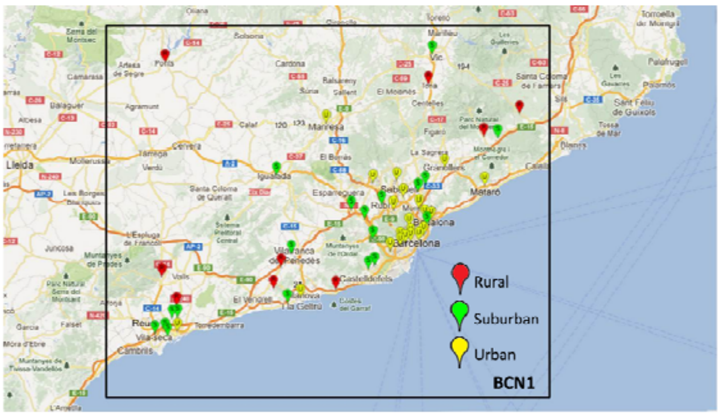

Figure 2. Air quality monitoring stations from the XVPCA located within the BCN1 domain. Coloured icons depict the type of area where the station is located.

Evaluation method

The comparison between both CALIOPE-AQFS grid resolutions over BMA is done in terms of gas-phase and aerosol concentrations (O_3, NO_2, SO_2 and PM10) at the lowest level. Modelled concentrations are compared against observations not validated from the Xarxa de Vigilància i Previsió de la Contaminació Atmosfèrica (XVPCA) providing Near Real Time (NRT) evaluation on an hourly basis. A number of 27 monitoring stations provide measurements to evaluate O_3, 40 for NO_2, 28 for SO_2, and 14 for PM10, respectively. Figure 2 shows the location of the XVPCA stations. The evaluation is based on the annual analysis of 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) and all stations (A). The study is performed over a natural year from September 1st 2011 to September 1st 2012, with a special focus on a pollution episode (from 3rd to 13rd October) representative of typical high-pressure condition in summer.

RESULTS

Annual evaluation

Figure 3 shows the annual mean concentration of O_3, NO_2, SO_2 and PM10 by station type. O_3 is the pollutant which presents the lowest impact with resolution increase. The rural group (3/27 stations) shows the highest sensitivity. However, this result is deviated by the Alcover rural station, located downwind the industrial emissions from Tarragona area, where the resolution increase improve the annual bias. NO_2 annual mean concentrations (underestimated in both resolutions) show high increments for urban stations. The resolution increase has the highest impact in SO_2 concentrations, mainly for urban stations where concentration increase ~3µgm^{-3}. The resolution increase has also a significant impact in PM10 annual concentration, decreasing concentrations (~3µgm^{-3}) in the same order of magnitude for all the station types.

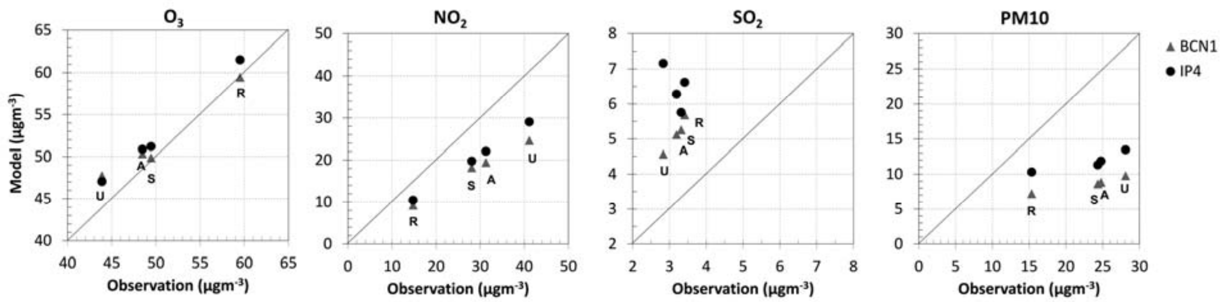

Figure 3. O_3, NO_2, SO_2 and PM10 annual mean concentration at two spatial resolution 4 km x 4km (IP4, black dots) and 1 km x 1km (BCN1, grey triangles) per station type (U = urban, S = suburban, R = rural, and A = all stations).

Table 1. Annual statistics for O_3, NO_2, SO_2 and PM10 concentration on an hourly basis at two horizontal resolutions 4 km (IP4) and 1 km (BCN1). N indicates the number of stations; % indicates the percentage of variability when resolution increases from 4 km (IP4) to 1 km (BCN1).

Station type		O_3				NO_2				SO_2				PM10			
		N	IP4	BCN1	%	N	IP4	BCN1	%	N	IP4	BCN1	%	N	IP4	BCN1	%
Rural	r	4	0.62	0.56	-9	6	0.26	0.36	37	4	0.06	0.05	-23	1	0.13	0.10	-22
Suburban		11	0.60	0.54	-9	18	0.39	0.42	6	16	0.04	0.04	22	9	0.25	0.24	-2
Urban		12	0.60	0.57	-5	16	0.41	0.47	13	8	0.04	0.02	-46	4	0.27	0.26	-4
All		27	0.60	0.56	-7	40	0.38	0.43	12	28	0.04	0.04	-6	14	0.25	0.24	-3
Rural	MB	4	2.0	0.2	-90	6	-4.4	-5.2	19	4	3.2	2.3	-29	1	-5.0	-8.1	60
Suburban		11	1.7	0.6	-64	18	-8.4	-9.8	18	16	2.4	1.9	-20	9	-13.0	-15.6	20
Urban		12	3.2	4.0	28	16	-12.1	-16.4	36	8	4.3	1.7	-60	4	-14.6	-18.2	25
All		27	2.4	2.1	-14	40	-9.2	-11.8	27	28	3.1	1.9	-37	14	-12.9	-15.8	22
Rural	RMSE	4	27.9	29.3	5	6	15.1	14.6	-3	4	16.7	17.4	4	1	16.4	17.0	4
Suburban		11	29.3	30.1	3	18	22.2	22.2	0	16	13.8	14.0	1	9	21.1	22.4	6
Urban		12	25.3	26.1	3	16	27.9	28.8	3	8	12.1	10.5	-14	4	22.4	24.8	10
All		27	27.3	28.2	3	40	23.4	23.7	1	28	13.7	13.5	-2	14	21.2	22.7	7

Table 1 summaries the annual statistics computed for both IP4 and BCN1 simulations. The grid effect is low for O_3 where MB decreases by 14% from 2.4 (4 km) to 2.1 (1 km) µg m^{-3} (< 1 µg m^{-3}). However, the resolution increase reduces annual mean correlation coefficients from 0.60 (4 km) to 0.56 (1 km). The urban stations are the exception, MB increase at traffic stations. On the other hand, NO_2 annual concentrations show an improvement based on spatial correlation coefficient from 0.38 (4 km) to 0.43 (1 km). However, the mean bias slightly increases by 27% (~3 µg m^{-3}) from 9.2 (4 km) to 11.8 µg m^{-3} (1 km). The resolution increase favours the model performance at rural stations where r increases from 0.26 to 0.36 and RMSE decreases by ~1 µg m^{-3}. SO_2, is the pollutant showing the lowest performance at both resolutions with large bias and very low r on an hourly basis. Several reasons could explain the low performance for SO_2, but the main reason for the model underestimations is related to the fact that emission are estimated based on the year 2004. In the present context, the resolution increase contributes to reduce MB by 37% (~3 µg m^{-3}) for all stations and by 60% (~2 µg m^{-3}) in urban stations. The impact on r is reduced, where r remain under 0.10. The resolution increase does not favour the PM10 model performance, the absolute MB increase by 22% (from 12.9 to 15.8 µg m^{-3}). This fact is significant for rural stations, where MB increases by 60%. The annual r shows low variability when increasing resolution with differences maximum differences about 0.03 at rural stations.

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. The increase of grid resolution contributes to reduce annual MB of SO_2 by 37 % and increase temporal correlation for NO_2 by 12%.

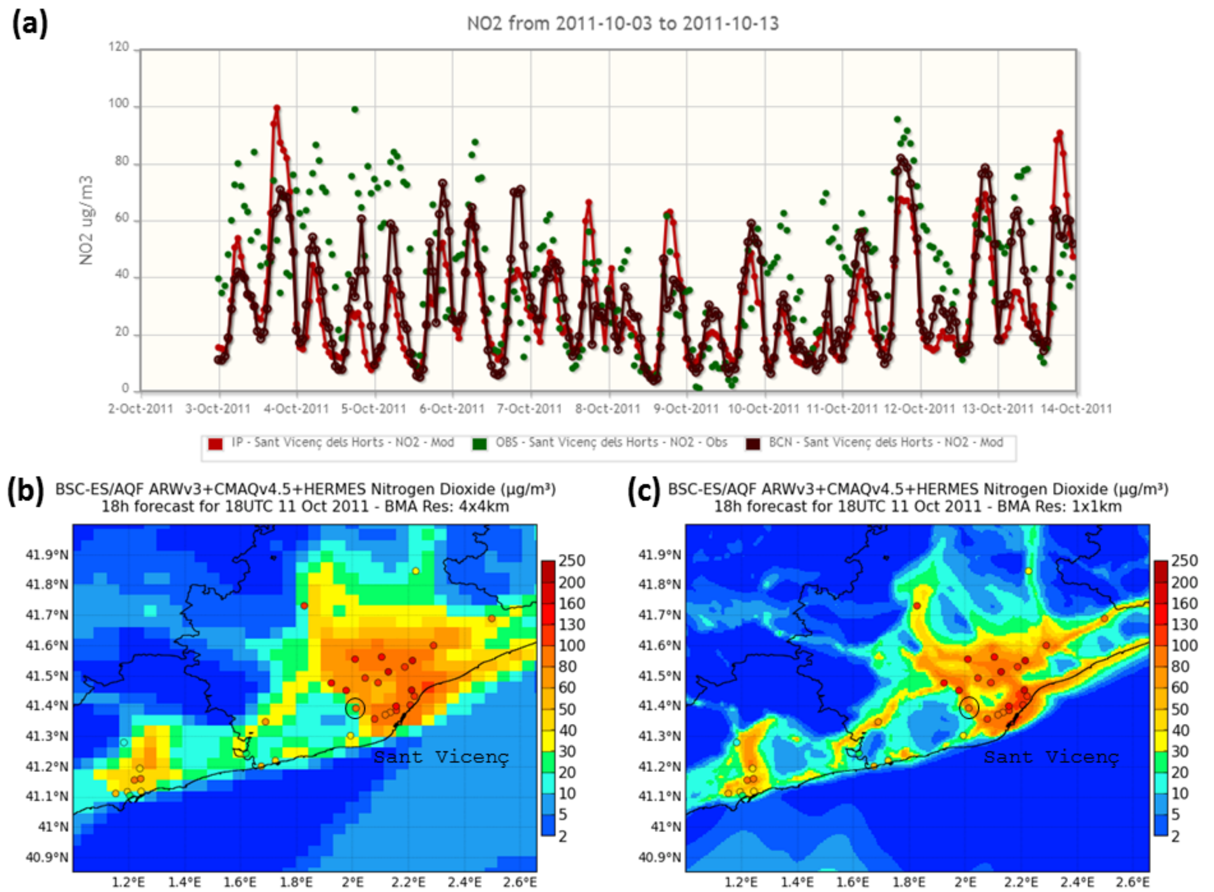

Figure 4. (a) NO_2 temporal series for the summer episode (3rd -13rd October) at Sant Viçent station for CALIOPE-AQFS at two resolutions: 4 km x 4 km (red line) and 1 km x 1 km (dark red line). Observations are green dots. (b and c) NO_2 modelled concentration maps versus observations (dots) at 18UTC for the resolution 4 km x 4 km and 1 km x 1 km, respectively.

Summer episode

The late summer episode (from 3rd to 13rd October 2011) is controlled by an anticyclone located over the western Mediterranean basin along with high isolation, allowing a weak synoptic forcing. Under this condition and together with a complex topography, the transport over BMA is dominated by sea breezes and mountain valley winds. The describe pattern is alternated with a frontal system (from 7th to 9th October) which inhibits the mesoscale circulation and leads precipitation events, contributing to reduce pollutant concentrations in air. Figure 4a shows observed NO_2 temporal series at the suburban station of Sant Vicenç during the summer episode compared with CALIOPE-AQFS at 4 km x 4 km (red line) and 1 km x 1 km (dark red line). NO_2 concentrations depict a remarkable daily cycle, since the station is located in a road connecting the city with industrial areas and is under the influence of traffic emissions. Differences between both resolutions are significant (~20 µgm^{-3}) in the afternoon peak (18 UTC) but there is not a clear tendency for model performance in terms of resolutions.

Figure 4a and b depicts NO_2 concentration maps for 18 UTC 11rd October 2011 at 4 km x 4 km and 1 km x 1 km, respectively. Overall, the definition of traffic roads significantly increases from 4 km to 1 km. In this sense, NO_2 concentrations at stations located near main suburban traffic roads (such as Sant Vicenç Sant Andreu, Martorell, Manresa and Sant Celoni) display a higher agreement at 1 km resolution than at 4 km. On the other hand, the resolution increase shows how the calculated concentrations increase in Barcelona downtown and the harbour from 80-100 µgm^{-3} (4 km) to 100-130 µgm^{-3} (1 km), allowing to allocate the peaks better than at lower resolution.

CONCLUSIONS

The present work shows the effect on increasing the horizontal resolution from 4 km to 1 km by means of a one-way nesting over the BMA in terms of air quality concentrations using the CALIOPE-AQFS. The results indicate that the horizontal grid influence highly depends on the environment (from urban to rural) and the studied pollutant. 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 based on annual correlation coefficient from 0.38 (4 km) to 0.43 (1 km). However, the mean bias slightly increases by 27% (~3 µg m^{-3}). Concerning SO_2, the resolution increase contributes to reduce annual MB by 37% for all stations and by 60% in urban areas. The increase of grid resolution is not favourable for O_3 and PM10 especially at rural stations. For O_3, spatial r decreases from 0.60 (4 km) to 0.56 (1 km) since O_3 is secondary formed downwind from VOC and NO_x sources. 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 resolution in terms of annual 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 during a typical pollution episode revels that NO_2 concentrations are better allocate at 1 km than at 4 km, increasing the concentration (~20 µg m^{-3}) in Barcelona urban conglomeration and the harbour with high agreement with observations. Based on the present results, the CALIOPE-AQFS provides forecast at 1 km x 1 km for Barcelona Metropolitan Area using the HERMESv2.0 which provides a more accurate and realistic emission than HERMES04 in terms of the current Spanish emission patterns based on methodology improvements and updated to the reference year 2009.

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