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IMPACT OF BOUNDARY AND INITIAL CONDITIONS ON NOx, NO_2 AND O_3 CONCENTRATIONS IN WRF-CMAQ SIMULATIONS OVER THE METROPOLITAN AREA OF BUENOS AIRES, ARGENTINA

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Abstract: In this work, we present a sensitivity analysis of nitrogen oxides (NOx), nitrogen dioxide (NO_2) and ozone (O_3) concentrations modelled with the Weather Research and Forecasting-Community Multiscale Air Quality Modelling System (WRF-CMAQ) in the Metropolitan Area of Buenos Aires (MABA) to initial and boundary conditions. Six configurations considering up to four nested modelling domains combined with two background O_3 concentrations (20 ppb and 30 ppb) are analysed. The model response to changes in these variables is investigated at two air quality monitoring stations and across the MABA. The WRF-CMAQ modelling system reproduces the temporal variations of NO_2 and NOx concentrations relatively well, with model errors varying between configurations, weeks and sites. While NOx concentrations are not sensitive to the background O_3 concentration, large differences are observed between three and four domains during a few hours, which appear to be due to differences in the wind field. NO_2 and O_3 concentrations depend on both the background O_3 concentration and the domain configuration, with the former having a greater effect in the spring week. On the other hand, the sensitivity simulations show different impacts across the MABA and an important role of power plants, which could be related to the height of the first model layer and need further analysis.

Key words: *boundary and initial conditions, Buenos Aires, nitrogen dioxide, sensitivity analysis, WRF-CMAQ.*

INTRODUCTION

The Metropolitan Area of Buenos Aires (MABA) is the third mega city in Latin America; however, observational studies of air quality in the area are scarce and only three monitoring stations are available. Most previous modelling studies in this area are based on different versions of an urban scale atmospheric dispersion model and present a relatively good performance (e.g., Venegas and Mazzeo, 2002; Pineda Rojas and Venegas, 2013). The implementation of a complex three dimensional chemical transport model such as the Community Multiscale Air Quality Modelling System (CMAQ, Byun et al., 2006), may contribute to study the role of sources that have not been considered previously (e.g., biogenic) and to perform process analysis which cannot be addressed with simpler models. However, it has been largely limited by the scarce air quality monitoring and the lack of detailed input data.

In a previous work (Luque et al., 2023), the Weather Research and Forecasting model (WRF, Skamarock et al., 2019) was implemented in the MABA at high spatial resolution (1 km), and the role of different physical schemes was studied focusing on meteorological variables that are relevant to air quality. Recently, we have implemented the WRFv4.2.1-CMAQv5.4 in this region for the first time. Given the large sensitivity of model results to boundary and initial conditions (BC/IC) found in other studies (e.g, Borge et al., 2010) and the need to understand the requirement of a large modelling domain in the MABA, in this work we perform a sensitivity analysis of nitrogen dioxide (NO_2), nitrogen oxides (NOx) and ozone (O_3) concentrations modelled with WRF-CMAQ to different BC/IC and modelling domain configurations. This includes three different domain set ups and two O_3 background levels. The objective is to find an adequate CMAQ configuration for the MABA.

METHODOLOGY

Six model configurations combining from one to four nested domains (**Figure 1**) with two O_3 background concentration levels ($[O_3]_b$), are analysed (see **Table 1**). Horizontal resolutions of domains D4 to D1 are 1 km, 3 km, 15 km and 45 km, respectively, with 80 vertical levels and 8 layers within the first kilometre. The selected $[O_3]_b$ values are 30 ppb (the default value in CMAQ) and 20 ppb based on previous studies (e.g., Mazzeo et al., 2005).

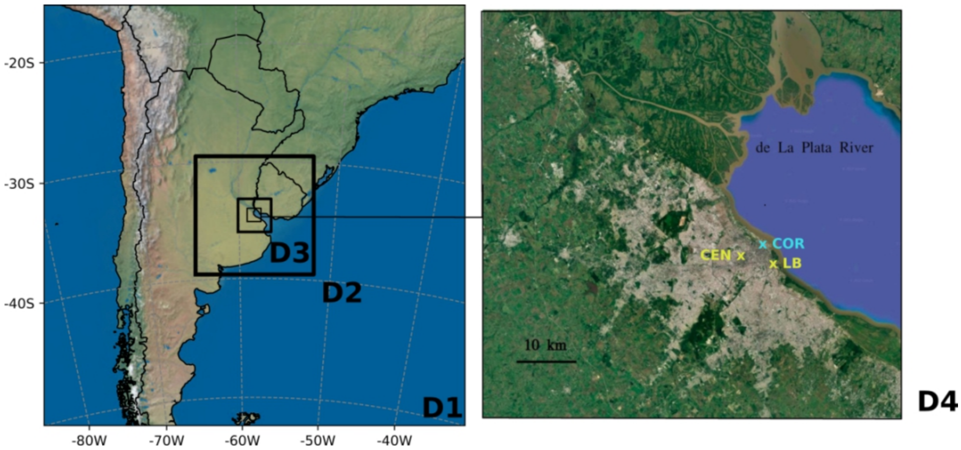

Figure 1. Four nested domains (left) and the innermost domain (right) with the air quality monitoring stations of Buenos Aires city: Parque Centenario (CEN, urban background), La Boca (LB, residential industrial) and Córdoba (COR, urban traffic).

All simulations use the same WRF physics schemes based on the results from Luque et al. (2023). CMAQ is run with the chemical scheme CB6r3. For the inner domain, a high resolution area source emissions inventory developed for the MABA (Venegas et al., 2011) and point sources data from JICA (2012) are used, while the EDGAR HTAPv2 emission inventory (Janssens-Maenhout et al., 2015) is considered for the other domains.

Table 1. Model configurations

Label	Planetary boundary	Surface layer	Land surface	Microphysics	Radiation	Urban	# Domains	$[O_3]_b$
stat_20ppb							1 / D4	20 ppb
stat_30ppb								30 ppb
dyn3_20ppb	BouLac	MM5	Noah	Thompson	RRTMG	SLUCM	3 / D2-D4	20 ppb
dyn3_30ppb								30 ppb
dyn4_20ppb							4 / D1-D4	20 ppb
dyn4_30ppb								30 ppb

The sensitivity of modelled hourly concentrations of NO_2 and NOx to the six model configurations from **Table 1** and their performance are assessed at two monitoring sites (CEN and LB) during one winter and one spring week. The sensitivity of O_3 concentrations is also analysed due to its chemical coupling with NO_2.

RESULTS

Modelled vs observed concentrations at CEN and LB

Figures 2 and 3 presents NOx and NO_2 modelled vs observed concentrations during each week at CEN and LB respectively. Between 50-90% of modelled results fall within a factor two of observations at both sites, depending on configuration. Correlations values are over 0.4 for almost all cases. At CEN, NO_2 concentrations are mostly overestimated and configurations with $[O_3]_b$ = 20 ppb (blue dots in **Figure 2**) present a better performance; while the opposite is observed at LB.

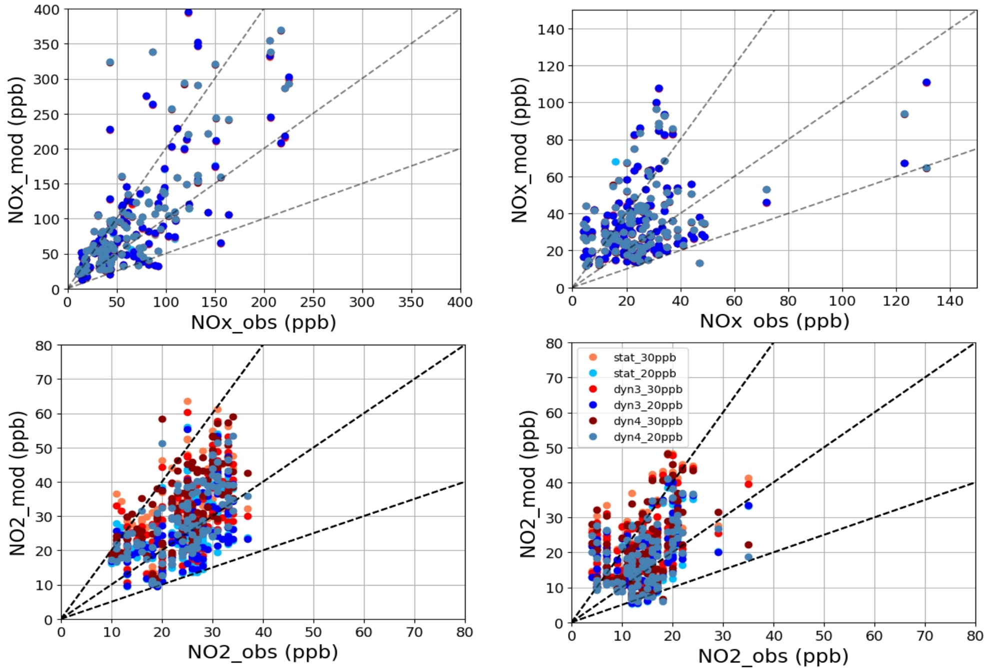

Figure 2. Modelled vs observed concentrations of NOx and NO_2 during the winter (left) and the spring (right) week at CEN.

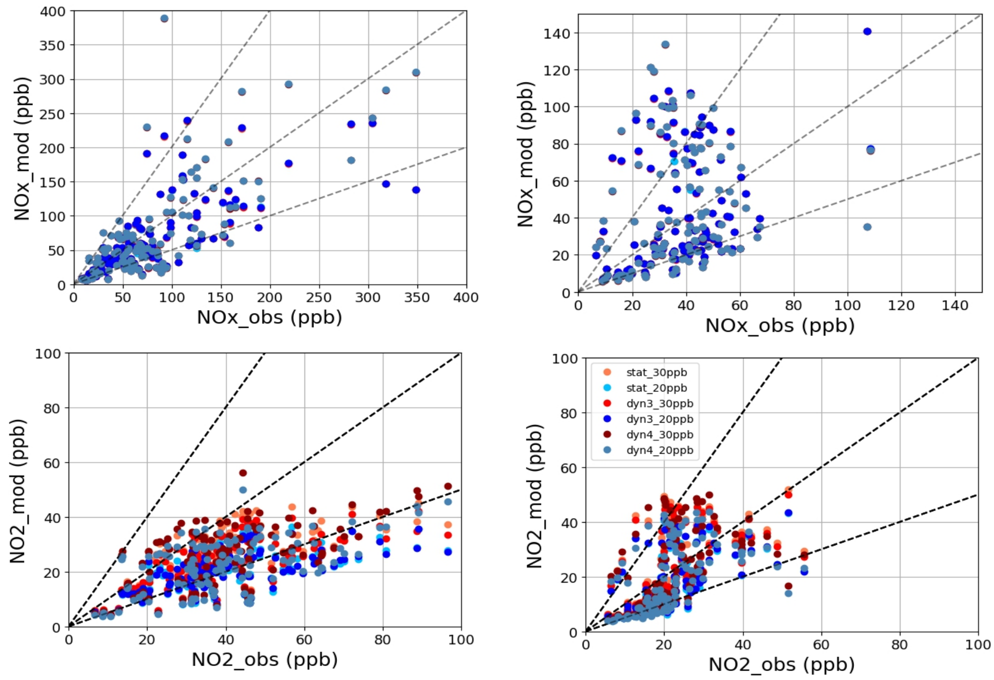

Figure 3. Modelled vs observed concentrations of NOx and NO_2 during the winter (left) and the spring (right) week at LB.

NOx concentrations are not sensitive to $[O_3]_b$ and present almost negligible differences between different modelling domains, except for a few hours during the winter week. The largest difference (+189 ppb) occurs between configurations dyn4 and the others. Since NOx does not depend on chemistry at the urban scale, such differences could be due to meteorology. At the time of the largest NOx concentration difference, at the receptor, a wind speed of 20% is obtained (0.88 m/s in 'dyn4' vs 0.73 m/s in 'dyn3' and 'stat'); while wind direction is 117° (SE) in 'dyn4' and 60° (NE) with 'dyn3' and 'stat' simulations.

As expected, NO_2 concentrations are higher with configurations having $[O_3]_b$ = 30 ppb (red dots in **Figure 2 and 3**) as these cases present higher O_3 availability for NO to NO_2 conversion. The hourly concentration ratios C30ppb/C20ppb are in the range 1.05-1.30 with greater differences around peaks (not shown). On the other hand, NO_2 concentration ratios for different domain set ups (Cdyn4/Cdyn3) vary between 0.41-2.10, with a greater effect in the winter week. For the modelled O_3 concentrations, C30ppb/C20ppb ratios vary between 1.10-3.60, while Cdyn4/Cdyn3 ratios are in the range 0.01-2.08.

Horizontal distributions of pollutant concentrations in the MABA

Figure 4 shows the distribution in the MABA of the modelled NO_2 concentration in the dyn4_20ppb scenario averaged over the winter week, its difference with that of the dyn4_30 ppb simulation and its difference with that of the stat_20ppb configuration. Higher mean NO_2 levels are observed to the north and west of the city due to prevailing winds from the SE in 'dyn4' simulations. The effect of background ozone is to increase the concentration over the whole MABA area, while the domain effect is more variable and seems to be due to changes in wind direction. In the spring week, a relatively higher contribution from point sources is observed, which is also noticed in the horizontal distribution of O_3 concentration (not shown) and needs further analysis. This could be due to the height of the first layer of the model (50 m) and/or higher mixing heights during the spring.

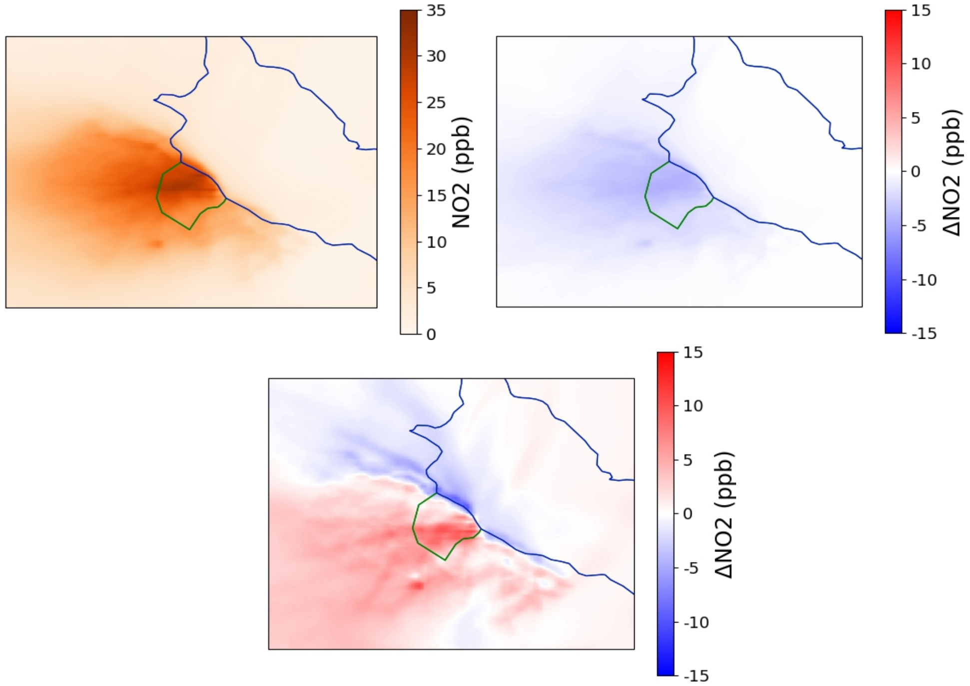

Figure 4. Mean NO_2 concentration in the winter week with configuration dyn4_20ppb (top left) and its differences with configurations dyn4_30ppb ('20ppb-30ppb', top right) and stat_20ppb ('dyn4-stat', bottom), in the MABA.

CONCLUSIONS

All tested WRF-CMAQ configurations present an acceptable performance to estimate NO_2 and NOx concentrations at two monitoring sites. The modelled NO_2 concentrations have a better performance at CEN with $[O_3]_b$= 20 ppb, which is consistent with a previously proposed value. On the other hand, the model performs best at LB with $[O_3]_b$ = 30 ppb, although this could be due to some underestimation of point sources close to the monitoring station and longer runs are needed to confirm this. NO_2 and O_3 modelled values are sensitive to both domain set up and $[O_3]_b$, with the latter having a greater effect on O_3 and mainly during the spring week. NOx is only sensitive to domain set up during a few hours due to differences in the surface wind field between configurations. On the other hand, the sensitivity simulations show different impacts across the MABA and an important role of power plants, which could be related to the height of the first model layer and need further analysis.

Finally, we have not found a single configuration presenting better performance for all cases (pollutants, sites and weeks). However, given that configurations with a background O_3 of 20 ppb perform better at the urban background site (CEN) which is less influenced by power plants emissions and that a larger domain is expected to better reproduce the regional O_3 concentration values, we conclude that the configuration with a background ozone value of 20 ppb and four nested domains is adequate for WRF-CMAQ simulations in the MABA.

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