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STATISTICAL EVALUATION OF THE URBAN ATMOSPHERIC DISPERSION MODEL DAUMOD-GRS TO ESTIMATE NO_2 CONCENTRATIONS USING NEW AVAILABLE DATA FROM BUENOS AIRES

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Abstract: In this work, a new statistical evaluation of the urban scale atmospheric dispersion model DAUMOD-GRS is presented considering four years (2009-2012) of surface hourly meteorological data and nitrogen dioxide (NO_2) concentrations from three air quality monitoring stations [representative of urban background (UB), urban traffic (UT) and urban industrial (UI) conditions] in the city of Buenos Aires. Statistical measures indicate that the performance of the model to estimate NO_2 concentrations in the city is reasonable, especially at the UB site. Additional simulations with different chemical settings show that modelled NO_2 concentrations are sensitive to the ozone background level. Potential model improvements include a variable ozone background concentration which needs to be assessed further considering the performance of the model to estimate ozone and nitrogen dioxide jointly.

Key words: *Buenos Aires, DAUMOD-GRS, model performance evaluation, model sensitivity, nitrogen dioxide.*

INTRODUCTION

DAUMOD-GRS is an urban scale air quality model that results from coupling the atmospheric dispersion model DAUMOD (Mazzeo and Venegas, 1991) and the simplified photochemical scheme GRS (Azzi et al., 1992). The description of the coupling can be found in Pineda Rojas and Venegas (2013). Unlike complex multi-scale models (e.g., Borge et al., 2018), DAUMOD-GRS allows long term (several years), high spatial (1 km^2) and temporal (1 h) resolution simulations at low computational cost, and that it does not require detailed input data to be operated.

DAUMOD-GRS has shown an acceptable performance to estimate hourly concentrations of nitrogen dioxide (NO_2) and ozone (O_3) at different sites of the Metropolitan Area of Buenos Aires (MABA) according to previous studies (e.g., Pineda Rojas, 2014). The measurements used in those evaluations come from short (2-3 weeks) monitoring campaigns carried out at several sites of the MABA. Recently, hourly NO_2 concentration data measured at three air quality sites were made available by the local environmental protection agency (APrA). These stations are considered as urban background (UB), urban traffic (UT) and urban industrial (UI), and allow a new and more detailed evaluation of the model considering a long record of observations. In this work, the performance of the DAUMOD-GRS model to estimate urban background NO_2 concentrations at these sites is assessed considering four years of observations. Since DAUMOD has been subject to extensive model evaluations for primary species (e.g., Venegas and Mazzeo, 2006), this work focuses on the role of the chemical scheme. Different simulations are performed in order to identify potential causes for discrepancies and options for future model improvements.

METHODOLOGY

Simulations are performed in a 85 km x 75 km domain considering hourly surface meteorological data (2009-2012)from the station located at the Domestic Airport and area source emissions of NO_x and VOC from the high resolution (1 km^2, 1 h) inventory developed for the MABA by Venegas et al. (2011). NO_x initial emission speciation is considered as 90% NO and 10% $NO_2$and that of VOC is based on the COPERT 4 (Ntziachristos et al., 2009) VOC speciation profiles relevant to the MABA vehicle feet composition. A constant regional background O_3concentration of 20 ppb is assumed according to the results of Mazzeo et al. (2005). For NO_x and VOCs, clean air levels are considered given that the MABA is surrounded by non-urban areas (Pineda Rojas and Venegas, 2013).

Modelled NO_2 hourly concentrations predicted at the grid cells where the three APrA air quality monitoring stations are located are stored and compared with the observed values using the BOOT package (Chang and Hanna, 2004) and the Openair software (Carslaw and Ropkins, 2012) through a set of common dimensionless statistics (NMSE: Normalized Mean Square Error, CORR: correlation factor, FA2: fraction of predictions within a factor of two of observations and FB: Fractional Bias) along with MEAN and SIGMA (standard deviation). The statistical comparison is performed considering modelled and observed values paired both in space and time, and different aggregation: i) by monitoring station, and ii) by diurnal/nocturnal hours. The model performance by ranges of wind speed and direction is also analysed. Finally, the model response to different chemical settings is assessed.

RESULTS

Considering all data (N=76336), observations and model results present mean NO_2 concentration values of 27.8 ppb and 27.2 ppb respectively. The statistics obtained from the comparison of observed and modelled NO_2 concentrations at the three stations are: NMSE=0.53, CORR=0.382, FA2=0.708 and FB=0.022. When considering the model results at the stations individually, slightly better results are obtained at the UB station (NMSE=0.39, CORR =0.469 and FA2=0.824), as expected. On the other hand, no significant differences are found in the statistics obtained for diurnal and nocturnal hours, although a higher correlation is found at night. On average, the DAUMOD-GRS model underestimates the NO_2 concentrations at daytime hours (FB=0.227) and overestimates them at night-time hours (FB=-0.131).

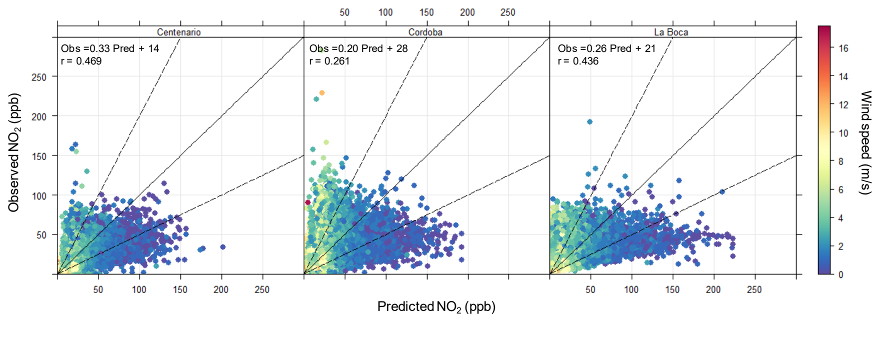

Figure 1. Scatter plot of modelled and observed NO_2 hourly concentrations at each air quality monitoring station.

Figure 1 shows how the model tends to overestimate NO_2 concentrations for wind speeds lower than 2 m s^{-1} and underestimates for wind speeds greater than 6 m s^{-1}. When considering the wind direction, the distributions of observed and modelled NO_2 concentration values obtained at Centenario (UB) are quite similar (Figure 2). At Córdoba (UT), the model produces a larger frequency of concentration values < 10 ppb with winds from the N-ESE and between 10-20 ppb with ESE winds; while some overestimation is observed with SW-NW directions. At La Boca (UI), a much greater frequency of NO_2 concentrations below 10 ppb is observed with winds coming from the N-ESE sector, suggesting that emissions at the highway Buenos Aires - La Plata could be underestimated. On the other hand, a greater occurrence of modelled concentration values above 50 ppb is observed with winds from the NW at the three monitoring sites.

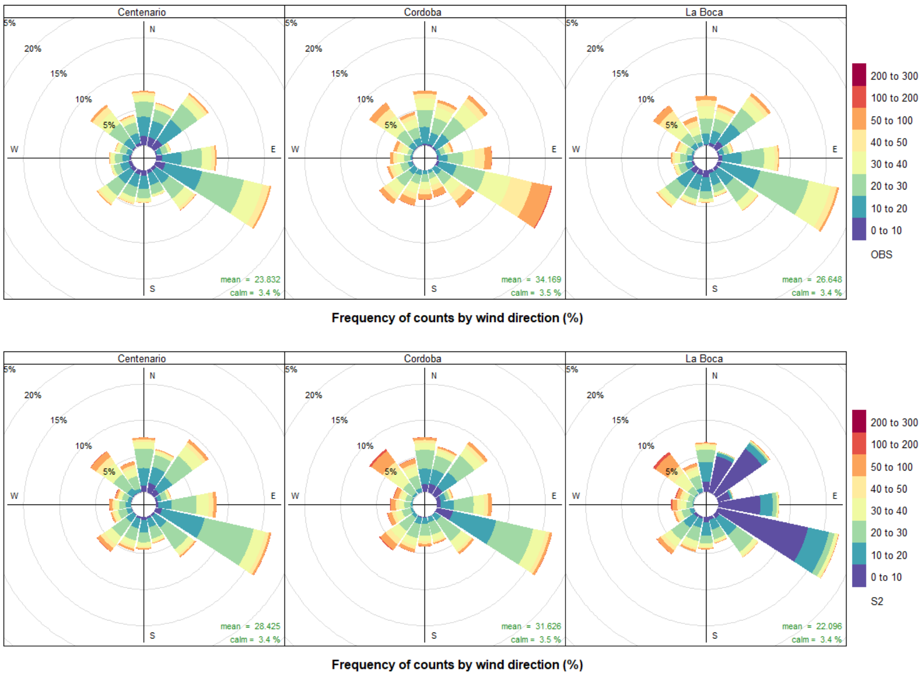

Figure 2. Distribution of observed (upper panel) and modelled (lower panel) NO_2 hourly concentrations by wind direction at each air quality monitoring station.

Figure 3 shows the mean hourly profiles of the observed and modelled NO_2 concentrations for each day of the week. At the three sites, larger differences are observed at the weekend when estimated NO_x and VOCs emissions (considering a typical workday hourly profile for the vehicular flux) are expected to be less representative of the real ones. At Centenario, the model overestimates the nocturnal values and the two daily maxima, and underestimates the concentrations at 10-16 h (local time). The night-time overprediction could be due to: i) an overestimation of the NO_x emission at the receptor, ii) an underestimation of the dispersion and iii) an overestimation of the NO_2 chemical formation; while the diurnal underprediction could be due to the opposite effects. A key input variable for the GRS is the initial O_3 concentration. In the DAUMOD-GRS model, this is given by the sum of its regional background level and the O_3 concentration remaining from the previous time step, computed at each receptor and time, and representing the "memory effect". This could also have an impact on such discrepancies based on previous analysis of model results.

At Córdoba and La Boca, the hourly mean nocturnal concentration values and the two maxima are in much better agreement with the observations and a larger difference is obtained at 10-16 h, compared to the results obtained at the UB site. Since Córdoba station is located in a street canyon, NO_2 concentration values estimated with DAUMOD-GRS are expected to be lower than the observed levels. In this sense, the agreement observed would be indicating that the model overestimates at night and early morning hours and underestimates during the day, as well as at Centenario. At La Boca site, the model slightly underestimates the two maxima. The NO_x emissions underestimation at or near this site, as suggested by Figure 2, could be compensated by the opposite effect at night-time hours.

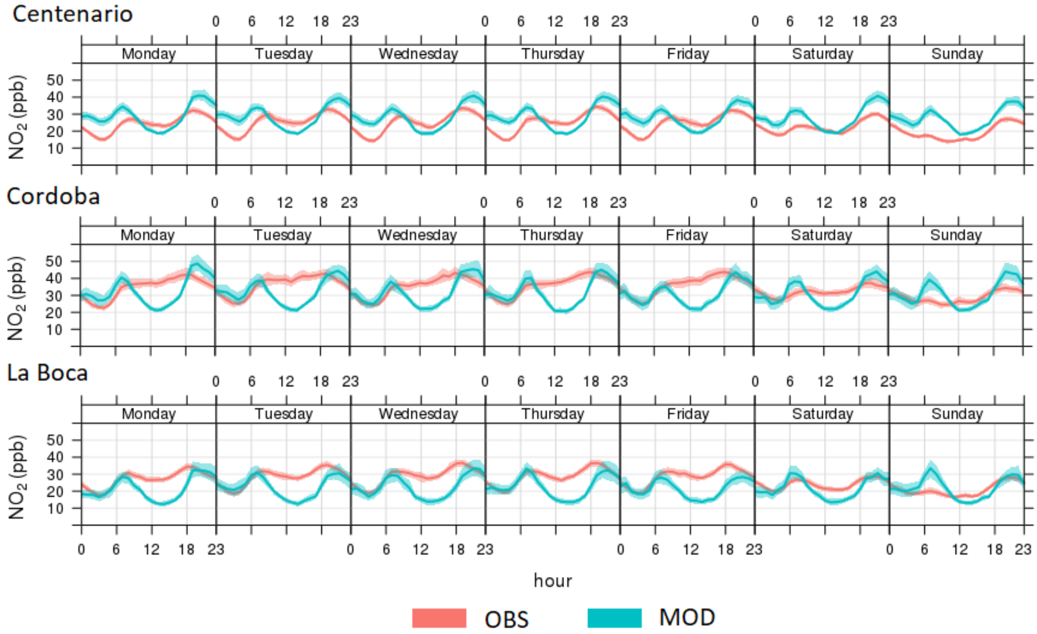

Figure 3. Hourly mean modelled and observed NO_2 concentrations at each air quality monitoring station. The shaded areas indicate the corresponding 95% confidence intervals.

Table 1. Statistics obtained from the comparison between modelled and observed NO_2 concentrations at each air quality monitoring station: Centenario (UB), Cordoba (UT) and La Boca (UI) [wo/CHEM: without chemistry, $[O_3]_r$: regional background O_3 concentration, wo/ME: without memory effect. MEAN and SIGMA in ppb. The standard simulation is highlighted].

Centenario (N=28093)	**MEAN**	**SIGMA**	**NMSE**	**CORR**	**FA2**	**FB**
OBS	24	12				
wo/CHEM	8	9	1.81	0.466	0.202	0.954
w/GRS ($[O_3]_r$ = 20 ppb)	28	17	0.39	0.469	0.824	-0.176
wo/ME	23	10	0.22	0.512	0.876	0.030
wo/ME & $[O_3]_r$ = 40 ppb	36	15	0.38	0.519	0.729	-0.393
Cordoba (N=22359)						
OBS	34	16				
wo/CHEM	12	13	2.05	0.253	0.199	0.967
w/GRS ($[O_3]_r$ = 20 ppb)	32	21	0.51	0.260	0.738	0.077
wo/ME	26	13	0.43	0.298	0.748	0.269
wo/ME & $[O_3]_r$ = 40 ppb	40	18	0.33	0.312	0.771	-0.152
La Boca (N=25884)						
OBS	27	13				
wo/CHEM	8	12	2.31	0.447	0.139	1.050
w/GRS ($[O_3]_r$ = 20 ppb)	22	22	0.73	0.437	0.556	0.187
wo/ME	17	14	0.63	0.438	0.559	0.418
wo/ME & $[O_3]_r$ = 40 ppb	26	21	0.53	0.432	0.556	0.027

In order to assess the effect of chemistry settings on the model performance, three additional simulations are run: 1) wo/CHEM: without chemistry; 2) wo/ME: standard run ($[O_3]_r$ = 20 ppb) without considering a memory effect; and 3) wo/ME and assuming a higher regional background O_3 concentration ($[O_3]_r$ = 40 ppb). Metrics from the statistical comparison between NO_2 observations and those obtained with each simulation are presented in Table 1. The poor performance of the model when the chemistry is turned off highlights the importance of its inclusion to simulate nitrogen dioxide concentration at these sites. The relatively good performance of the standard simulation supports the fact that a highly simplified photochemical scheme as the GRS may be enough to estimate NO_2 at these sites. When removing the memory component from the model, a slight improvement is obtained in the metrics at the three sites except for FB that worsens at Cordoba and La Boca (Table 1). By stratifying the data in diurnal/nocturnal hours, it is found that this improvement is greater at night (not shown). Finally, when a higher regional ozone concentration level is considered (double), a change greater than 50% (compared with that of the standard simulation) is obtained in the modelled mean NO_2 concentration values. These results show that the model is quite sensitive to this variable.

CONCLUSIONS

The metrics obtained from the statistical comparison of modelled hourly NO_2concentrations with those observed at the three air quality monitoring sites of the city of Buenos Aires, are within acceptable ranges. The results contribute to confirm that the performance of the DAUMOD-GRS to estimate NO_2 concentrations in the city of Buenos Aires is fair, with a slight tendency to overestimate the night-time values and underestimate the diurnal ones. As expected, the model performs best at the urban background station.

Differences in the modelled and observed concentration distributions by wind direction suggest that NO_x emissions could be overestimated to the SW-NW sector of the UT site and underestimated to the N-ESE of the UI station. Additional runs carried out with the aim of analysing the roles of the chemical module and the memory effect, show an improvement in the statistical measures when the memory component is removed from the simulations (mainly at night-time hours). On the other hand, NO_2 concentrations estimated with DAUMOD-GRS appear to be quite sensitive to the regional ozone background concentration at the three sites. Therefore, potential model improvements in DAUMOD-GRS could also result from either an update of the emissions inventory (including temporal profiles for non-working days and local-specific NO_2/NO_x ratios) and/or a better estimate/adjustment of the ozone regional background concentration presumably by means of space and time-variant profiles. Future model evaluations of the DAUMOD-GRS model to estimate ozone considering such changes will help to determine it.

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