EXTENDED ABSTRACT

Evaluating simple and complex models for urban NO$_2$ concentrations: DAUMOD-GRS and WRF-CMAQ in Buenos Aires

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Abstract

We compare urban NO$_2$ concentrations obtained with a simple semi-empirical model (DAUMOD-GRS) and a complex modelling system (WRF-CMAQ) over the Metropolitan Area of Buenos Aires, using a 1km resolution NOx and VOC emission inventory and consistent boundary assumptions for July and November 2012. Model performance is acceptable at three sites and better in winter at the urban background station. Both models capture hourly variability, but NO$_2$ underestimations occur at industrial residential sites under NNW–N winds without corresponding NOx errors, suggesting missing upwind background contributions. Sensitivity tests to key parameters show similar responses in both models, except for the emitted NO$_2$/NOx fraction that mainly affects DAUMOD-GRS. WRF-CMAQ simulations including all available emission sources and four nested domains improve performance at the residential industrial sites with ENE-ESE winds in spring, highlighting the influence of power plants. Finally, monthly mean fields are broadly similar, though DAUMOD-GRS yields higher maxima and stronger gradients. Comparisons with passive sampling campaigns could help assess each model's ability to reproduce spatial NO$_2$ gradients in urban areas.

Introduction

Air quality models can be classified as simple or complex: simple models, based on semi-empirical transport and dispersion formulations, allow multi-year simulations with low input data and computational resources, while complex models represent detailed physical and chemical processes, requiring larger inputs, greater computational cost, and specialized expertise. Comparing both model types under common conditions may help identify the role of processes absent from simpler ones and determine when these are sufficient. DAUMOD-GRS (Pineda Rojas and Venegas, 2013) is an urban scale atmospheric dispersion model that estimates nitrogen dioxide (NO$_2$) and ozone (O$_3$)

concentrations in the Metropolitan Area of Buenos Aires (MABA), the third largest mega-city in Latin America. On the other hand, the WRF-CMAQ modeling system has been recently implemented in the region using four nested domains with a 1km resolution in the inner domain (Luque et al., 2025).

MABA has three permanent monitoring stations [Parque Centenario (CEN), Córdoba (COR), and La Boca (LB)] plus a former site Dock Sud (ACU) outside the city. The scarce monitoring and the lack of long-term O_3 measurements limit a comprehensive evaluation of the DAUMOD-GRS chemical module, although previous assessments have shown good performance of the model for estimating NO_2. Other studies applying clustering methods have contributed to improve our understanding of model solutions across the region (e.g., Pineda Rojas et al., 2025). Here, we compare DAUMOD-GRS and WRF-CMAQ simulations for two months of 2012 at three sites, and throughout the MABA, using similar emission and boundary conditions (WRF-CMAQ with one domain and only area sources) and considering full WRF-CMAQ simulations with four nested domains and regional, biogenic, and power plant emissions. The aim is to evaluate DAUMOD-GRS against a widely used complex model and to explore the influence of processes and sources not addressed in earlier studies.

Models descriptions and analysis

Air quality models

DAUMOD-GRS is a steady-state atmospheric dispersion model which includes simplified chemistry to represent the VOC–NO_2–O_3 interactions (Pineda Rojas and Venegas, 2013). It has a modular and sequential structure where pollutants are first transported and dispersed, and can then react following a seven reaction scheme and a variable reaction time based on the residence time of the species from contributing sources.

The WRF-CMAQ modeling system implemented in the MABA, with the specific configuration used described in Luque et al. (2025), combines the WRF4.2.1 meteorological model with the CMAQ5.4 chemical transport model. The configuration includes a single-layer urban parameterization and the cb6r3 chemistry mechanism.

Analysis and data

Two 2012 periods were selected: 16 July–11 August (winter) and 5 November–1 December (spring), each with a two-day spin-up. In the first part of the study, both models were applied in the MABA using only NOx and VOC area source emissions (Venegas et al., 2011) at 1 km resolution. WRF-CMAQ used a single 1 km domain; both models assumed clean air concentrations and a static 20 ppb O_3 background. Sensitivity analyses were performed for two parameters: f-NO_2 (0.10–0.15) and background O_3 (20–40 ppb). In the second part, WRF-CMAQ was run with the same

base setup but four nested domains (45, 15, 3, 1 km) including biogenic, power plant, and regional (EDGAR) emissions, as included in Luque et al. (2025).

We refer to simulations as: DAUMOD, CMAQ (1 domain) and CMAQ_all (4 domains and all sources). All hourly NO_2 outputs were compared to observations at three sites: CEN (urban background), LB (residential industrial), and ACU (residential industrial). Model performance was evaluated using FB, NMSE and FA2 (Chang and Hanna, 2004). Time series and horizontal fields of NOx and O_3 were also analyzed to support interpretation of results.

Results

DAUMOD vs CMAQ (1-km domain, area sources only): Across both months and sites, performance metrics fall within acceptable ranges for NO_2, with better skill in winter and at CEN. At CEN (winter), DAUMOD achieved FB = −0.06, NMSE = 0.14, FA2 = 0.94, r = 0.45, while CMAQ reached FB = −0.02, NMSE = 0.25, FA2 = 0.92, r = 0.40. Both models reproduce hourly NO2 variability, although in winter, CMAQ more often overestimates peaks under low wind (**Figure 1**), while in spring DAUMOD overestimates some peaks more than CMAQ (not shown). During some days, both models considerably underestimate NO_2 concentrations at LB (and, to a lesser extent, ACU) without a comparable error in NOx, coinciding with NNW–N winds which suggest an unrepresented urban background contribution near those sites.
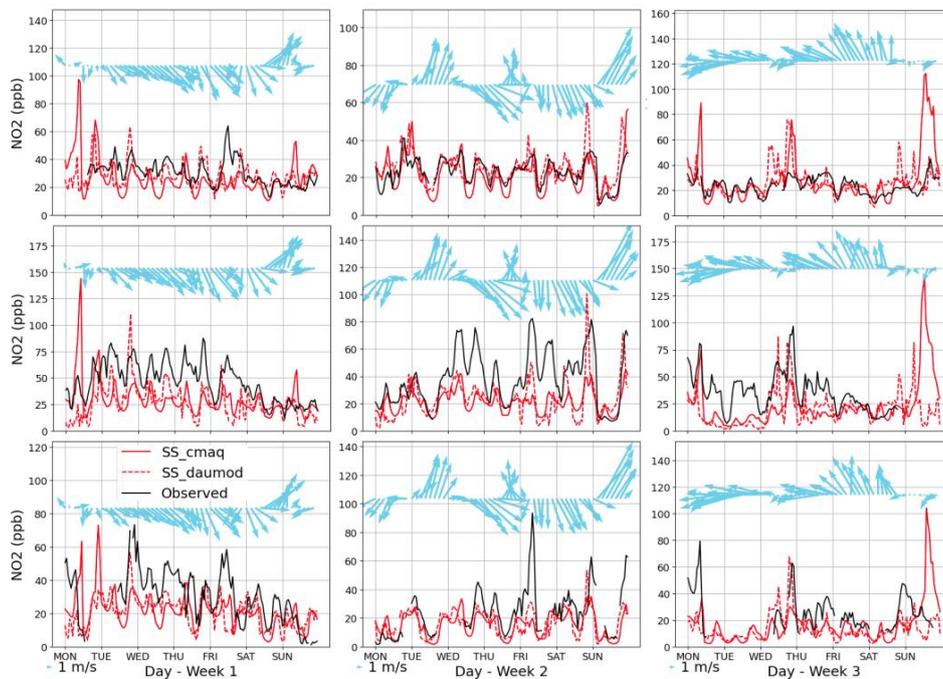

Figure 1: Hourly NO_2 concentrations at each monitoring site during the winter month, observed (black) and modeled (red) with DAUMOD-GRS and WRF-CMAQ for a single-domain simulation with area source emissions only. Hourly modeled wind vectors are shown in light blue.

Sensitivity to key parameters: Both models are highly sensitive to background O_3, increasing NO_2 as O_3 background is raised, with the strongest impact on peaks. Sensitivity to the fraction of NO_2 in total NOx differs: CMAQ responds weakly, whereas DAUMOD shows a noticeable response. Neither parameter adjustment resolves the large NO_2 underestimations at LB during periods dominated by NNW–N (and ENE–ESE) winds.

Horizontal fields (monthly means): Both models produce similar spatial patterns, but DAUMOD yields higher maxima and stronger horizontal gradients for NOx and NO_2 and lower O_3; domain-wide winter monthly-mean NO_2 maxima reach 33 ppb (DAUMOD) vs 25 ppb (CMAQ). These differences may affect estimation of exceedance areas. They could reflect larger vertical mixing and/or advection representation in CMAQ relative to DAUMOD.
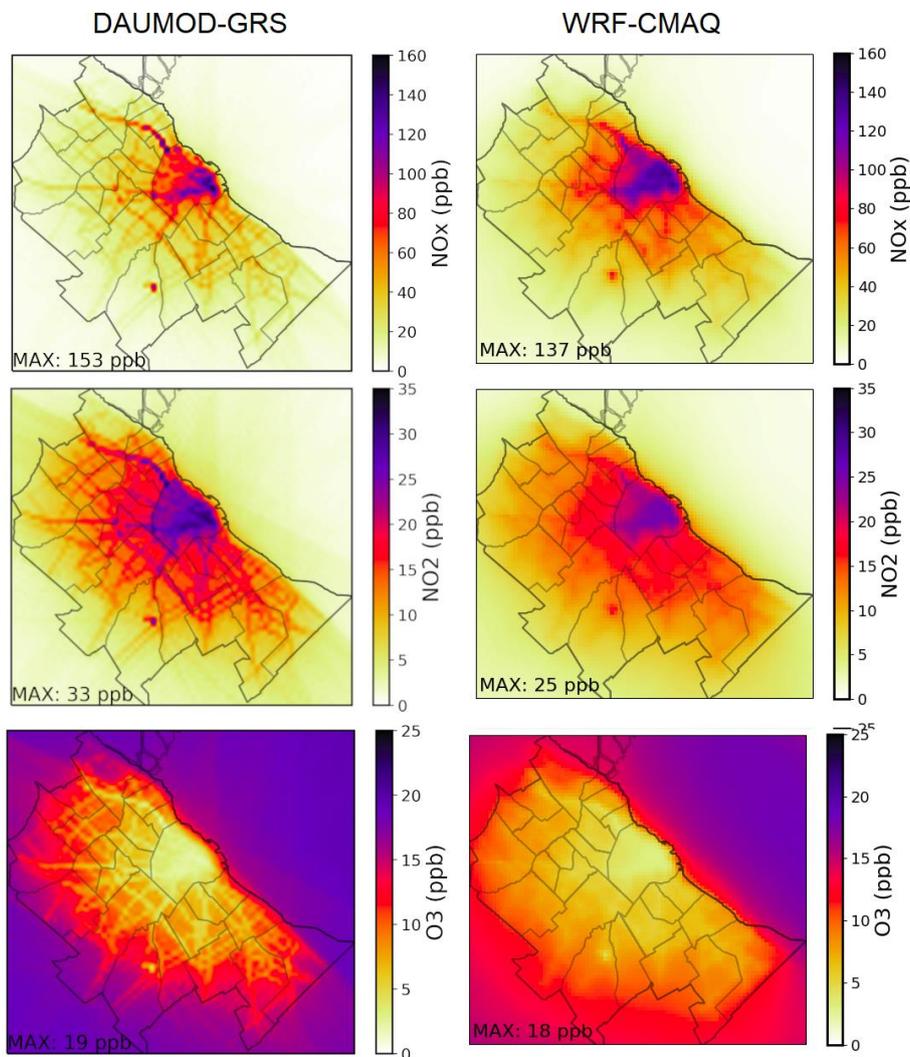

Figure 2: Mean concentrations of NOx, NO_2, and O_3 in the MABA during the winter month, estimated with DAUMOD-GRS (left) and WRF-CMAQ (right) under similar emissions and boundary assumptions.

Full CMAQ configuration (CMAQ_all: 4 domains + biogenic + point + regional): In winter, differences relative to the 1-domain simulation are small, with a slight improvement at LB under NE winds. In turn, in spring, CMAQ_all improves NO_2 peaks under ENE–ESE winds (highlighting power plant contributions), but underestimations persist under NNW–N winds, pointing to underestimated sources from the NNW–NW sector in the vicinity of LB and ACU. Spatially, winter maps change little; spring maps show localized increases near the coast where the power plants are located.

Conclusions

Both DAUMOD and CMAQ (1 km, area sources only) meet common performance benchmarks for NO_2, showing better performance at the urban background site (CEN) in the winter month. Large underestimations occur at LB (and ACU) under NNW–N winds, suggesting missing urban-background contributions from upwind sectors. Sensitivity analyses show that background O_3 strongly influences NO_2 peaks in both models, while the NO_2/NOx emission fraction mainly affects DAUMOD; however, neither parameter explains the LB underestimations. Although spatial patterns are broadly similar, DAUMOD produces somewhat higher NO_2 and NOx maxima (and lower O_3) and steeper gradients than CMAQ, which may influence exceedance area assessments. Adding biogenic, point, and regional contributions in CMAQ slightly improves agreement under certain wind sectors (ENE–ESE in spring) but does not resolve the NNW–N underestimations, suggesting underestimated sources in that direction.

References

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