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ANALYSING CONDITIONS LEADING TO HIGH NO_2 CONCENTRATIONS SIMULATED WITH THE DAUMOD-GRS MODEL IN A CONTEXT OF SCARCE MONITORING DATA

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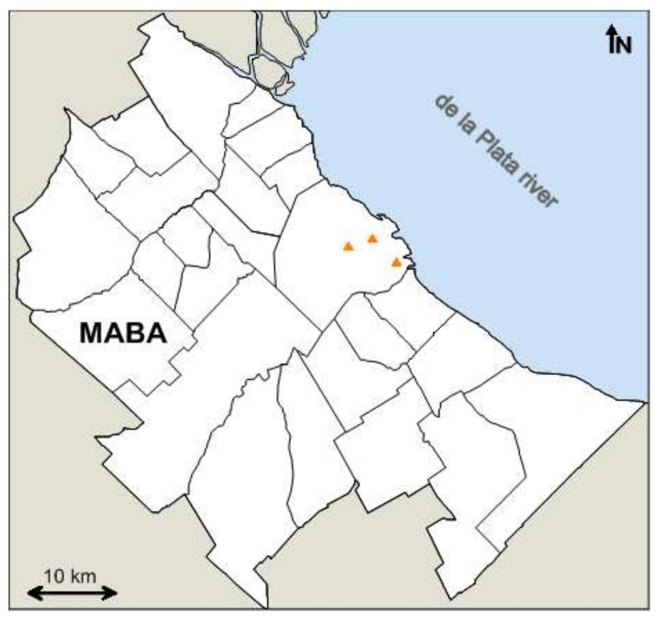
MOTIVATION & OBJECTIVES

Metropolitan Area of Buenos Aires (MABA)



(3,830 km², +15,000,000 inhab.)

Air quality monitoring stations in the city of Buenos Aires

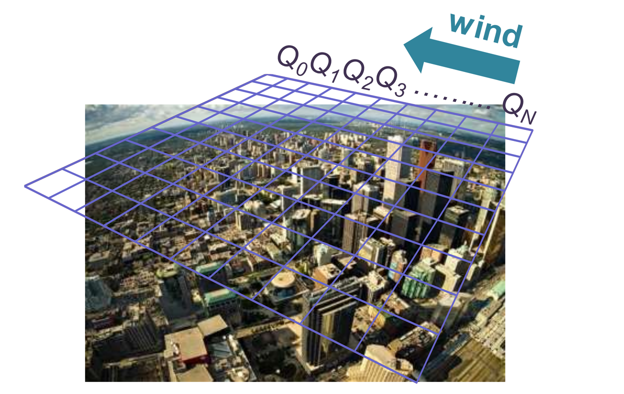
CEN: urban background
COR: urban traffic
LB: residential industrial

DAUMOD-GRS [1] is an urban-scale atmospheric dispersion model that shows acceptable performance in estimating the hourly concentration of nitrogen dioxide (NO_2) [2]. Given the few air quality monitoring sites in the MABA, there is a need to have a good understanding of the model results at locations other than the stations. In this work, we analyse both input and output (I/O) variables at the time of occurrence of relatively high hourly NO_2 concentrations to study the solutions of the DAUMOD-GRS in the MABA. The role of chemistry on NO_2 events is further explored performing a sensitivity analysis to key parameters. The aim is to understand the behaviour of the model across the metropolitan area in order to improve its performance in a context of scarce air quality data.

THE DAUMOD-GRS MODEL

DAUMOD [3]

- Based on the two-dimensional diffusion equation
- Developed for **area sources of intensity Q_i**
- The **x-axis** is in the **mean wind direction**



$$C = a\,[\,Q_0\,x^b + \sum_{i=1}^{N}(Q_i - Q_{i-1})(x - x_i)^b\,] \,/\, (|A_1|\,k\,z_0^b\,u_*)$$

GRS [4]

Interaction between NO_x-VOCs-O_3

ROC + hv → ROC + RP
RP + NO → NO_2
NO_2 + hv → NO + O_3
NO + O_3 → NO_2
RP + RP → RP
NO_2 + RP → SGN
NO_2 + RP → SNGN

ROC: all VOCs species
RP: all radicals
SGN: stable gaseous nitrogen
SNGN: stable non-gaseous nitrogen

METHODOLOGY

1. Conditions of the simulations

- DAUMOD-GRS is applied over the MABA considering:
  - Four years (2009-2012) of surface hourly meteorological data from the domestic airport (✈)
  - NOx and VOCs area source emissions from the high resolution (1km x 1km) emissions inventory developed by Venegas et al. [5].
  - Clean air concentration values as regional background levels.
- For each NO_2 event: [NO_2] > 106 ppb [6], the I/O variables are stored.

2. Clustering of NO_2 events

- A k-means algorithm is applied considering as classification variables:

Hour (H), NO_2 concentration ([NO_2]), wind speed (WS), wind direction (WD), air temperature (T), sky cover (SC), total solar radiation (TSR), NO_2/NOx concentration ratio (ratio), atmospheric stability class (KST), etc.

- An appropriate number of clusters (k) is obtained by analysing solutions for different values of k.
- The differences between the clusters in the conditions of the events are analysed.

3. Standard (SS) and sensitivity simulations (S1-S4)

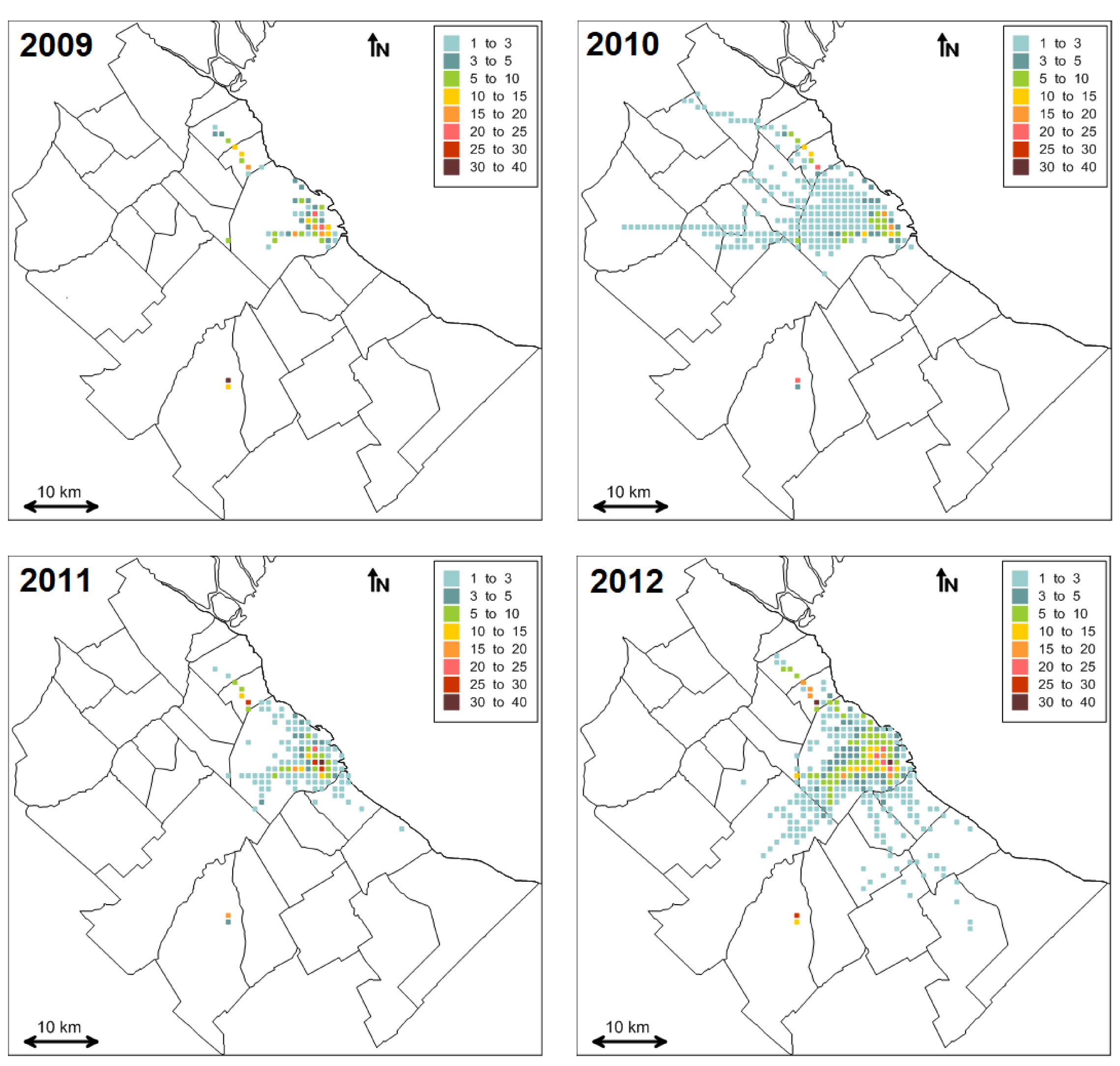
- Key parameters for the chemical module (GRS):
  - Δt_r: reaction time,
  - f-NO_2: fraction of NO_2 in the NOx emission,
  - $[O_3]_r$: regional background O_3 concentration.

Simulation	Parameter		
	Δt_r	f-NO_2	$[O_3]_r$
SS	variable	0.10	20 ppb
S1	60 min		
S2	variable	0.15	
S3		0.10	30 ppb
S4			40 ppb

RESULTS

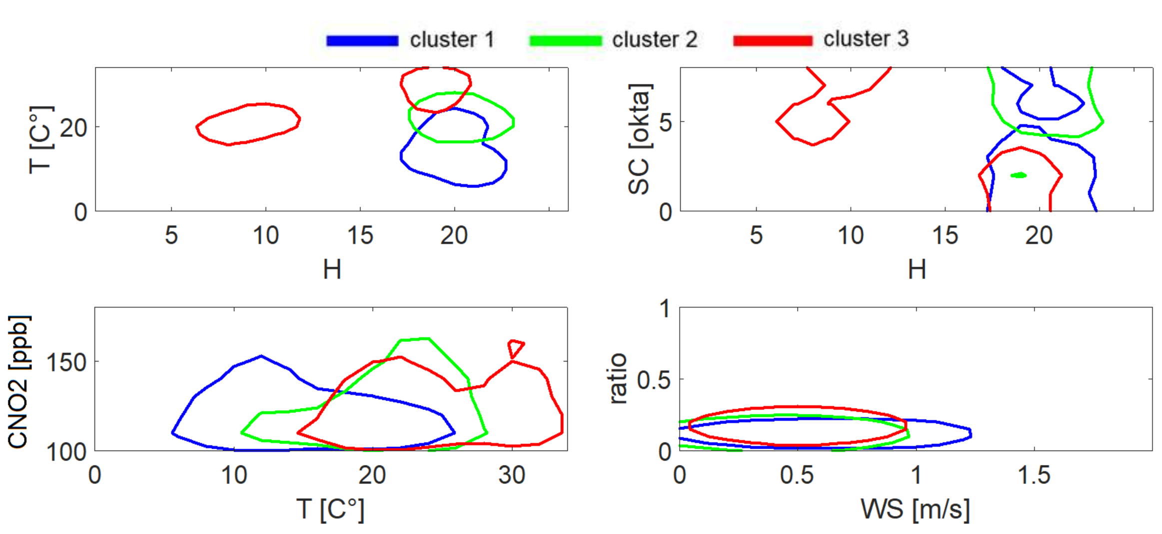
1. NO_2 events in the MABA (2009-2012)

Number of hourly NO_2 concentrations above 106 ppb per year in the standard simulation (SS)

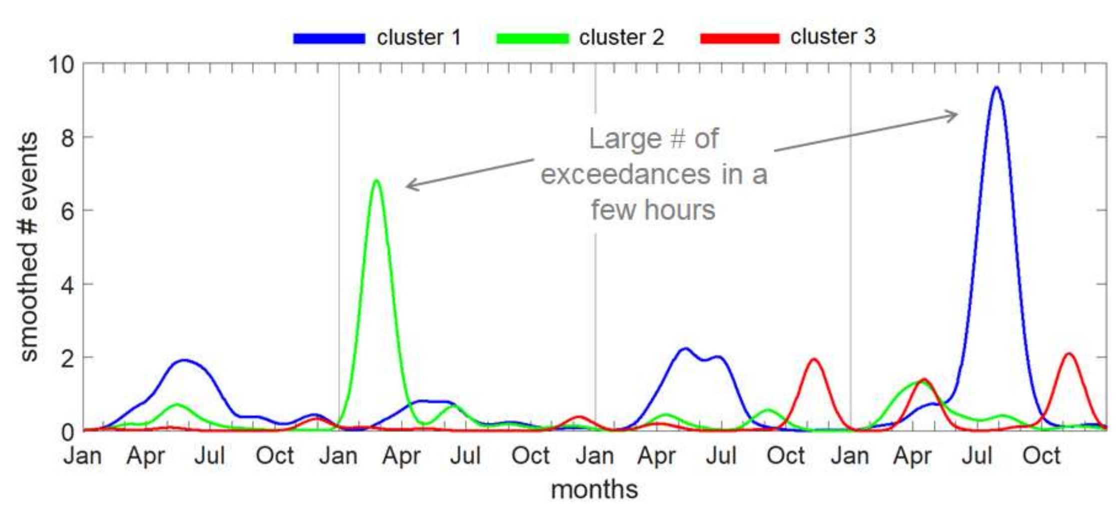


2. Conditions leading to NO_2 events

Curves containing 90% of the objects in each cluster over different values of the I/O variables



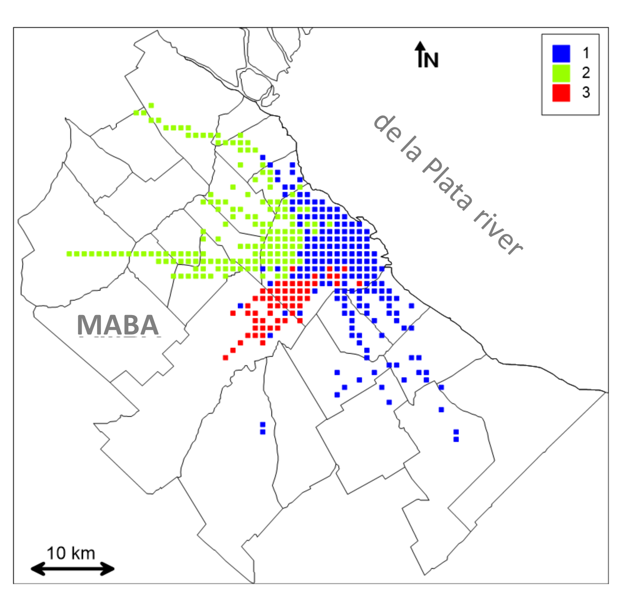
Smoothed distribution over time of number of NO_2 events of each cluster



Distribution of the dominant cluster

Cluster 2
Events occur in the afternoon-evening with higher SC, E and NNE winds

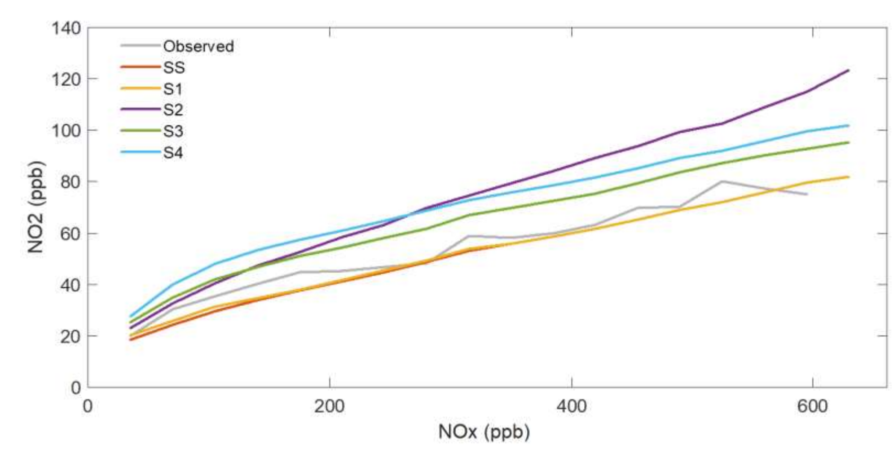
Cluster 3
Events occur in the morning with moderate T and high SC or in the evening with high T and low SC. w/ NE winds and slightly higher ratios



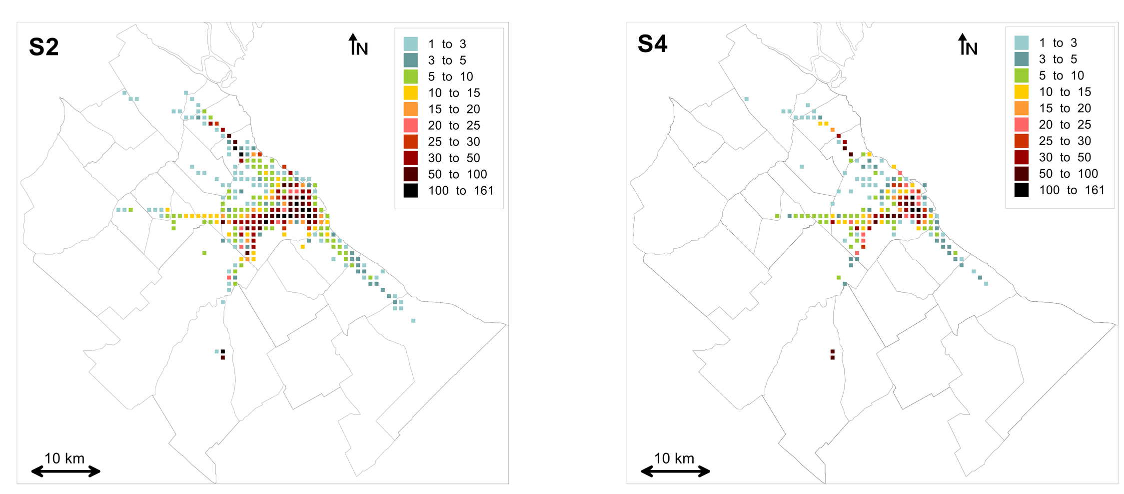
Cluster 1
Events occur in the afternoon-evening with lower T and SC, W and NNW winds, and higher WS range.

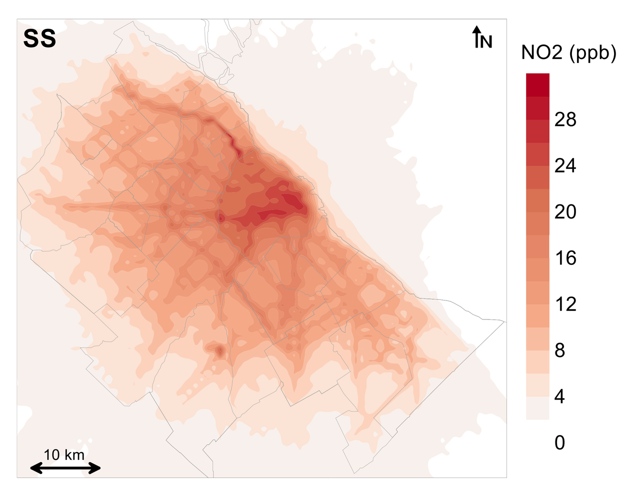
3. Sensitivity to key model input parameters

Average NO_2 vs. NOx concentrations for each sensitivity simulation at CEN (UB) station



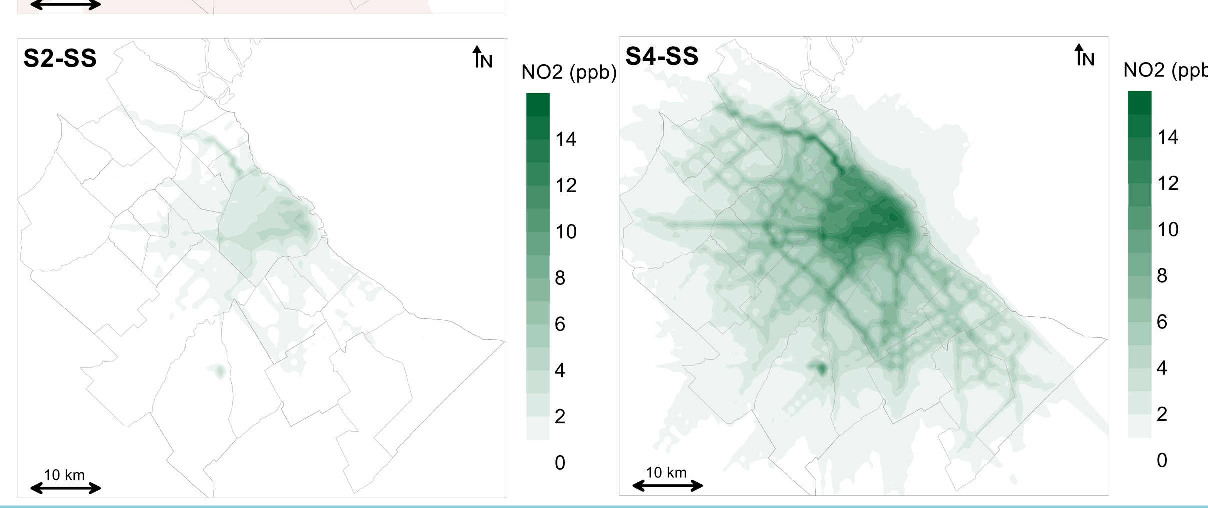
Number of NO_2 events in 2009, in simulations S2 and S4





NO_2 annual concentration in 2009

	SS	S2	S4
Max freq. hourly events (events/yr)	36	160	108
Area of events (km^2)	52	289	172
Highest annual conc. (ppb)	29	34	44
Area of events (km^2)	2423	2510	2988



CONCLUSIONS

- Over a period of four years, N=2335 events were obtained and can be described by three clusters.
- The temporal distribution of the clusters revealed a change in the reporting of low WS values from 2010 onwards, leading to an overestimation in the area of exceedances.
- The conditions leading to NO_2 events are variable, except for the NO_2/NOx concentration ratio, which is low (< 0.2) for all clusters.
- Simulations of sensitivity to key parameters for chemistry showed a small effect of Δt_r, while f-NO_2 and $[O_3]_r$ significantly affected NO_2 events highlighting the importance of their estimation.
- Analysis of the conditions leading to high concentrations of NO_2 can provide information on the behaviour of the model, which may be particularly useful in locations with poor air quality monitoring, such as MABA.

REFERENCES
[1] Pineda Rojas, A.L. and Venegas, L.E., 2013: Upgrade of the DAUMOD atmospheric dispersion model to estimate urban background NO_2 concentrations. Atmos. Res., 120-121 147-154.
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