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CLUSTERING OF ATMOSPHERIC AND EMISSION CONDITIONS THAT LEAD TO MODELLED PEAK OZONE CONCENTRATIONS

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MOTIVATION AND OBJECTIVES

An application of a simple urban air quality model (DAUMOD-GRS, [1]) shows that summer maximum O_3 hourly concentrations (C_{max}) above 40 ppb [one of the accepted thresholds to protect vegetation] occur outside the Metropolitan Area of Buenos Aires (MABA) where the absence of observations impedes model testing [2]. In addition, those relatively high values present the greatest model uncertainty caused by possible errors in model input variables [3]. In this context, a probability assessment of such exceedances may provide a more robust estimate than a deterministic one.

This work presents a Monte Carlo (MC) evaluation of the probability of occurrence of peak O_3 hourly concentrations greater than 40 ppb in the MABA during a typical summer season, using the DAUMOD-GRS model. In order to overcome the limitations due to the size of the MC outcomes, a clustering analysis is performed aiming to identify the environmental conditions under which C_{max} occurs and to gain insight on the model performance outside the MABA, where the highest values are obtained.

METHODOLOGY

The DAUMOD-GRS model

DAUMOD-GRS is an urban-scale atmospheric dispersion model which allows estimation of ground-level urban background concentrations of NO_2 and O_3 resulting from area source emissions of NO_x and VOCs. Its performance evaluation in the MABA is discussed in [1] and [2].

Base case conditions

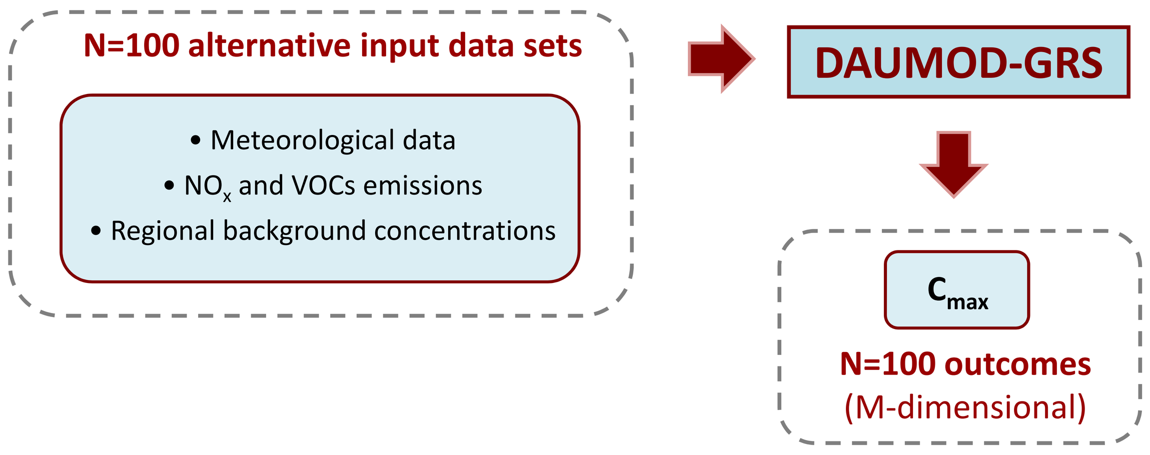
- Surface hourly and sounding meteorological data from a typical summer (2007)
- MABA area source emissions of NO_x and VOCs
- Clean air regional background concentrations

Probabilistic evaluation of C_{max} > 40 ppb

Probability density functions (N: normal, LN: lognormal) and uncertainty ranges of the model input variables [4]

Input variable	PDF	2σ / E(%)
WS (%)	LN	30
DIR (°)	N	30
T (°C)	N	3
SC (okta)	N	1
KST	N	1
TSR (%)	LN	12.5
QNO_x (%)	LN	40
QVOC (%)	LN	80
$[O_3]_r$ (%)	LN	30

MC simulations:



➔ $P(C_{max}>40\ ppb)$ = No. of exceedances / N

Clustering analysis of the Monte Carlo outcomes

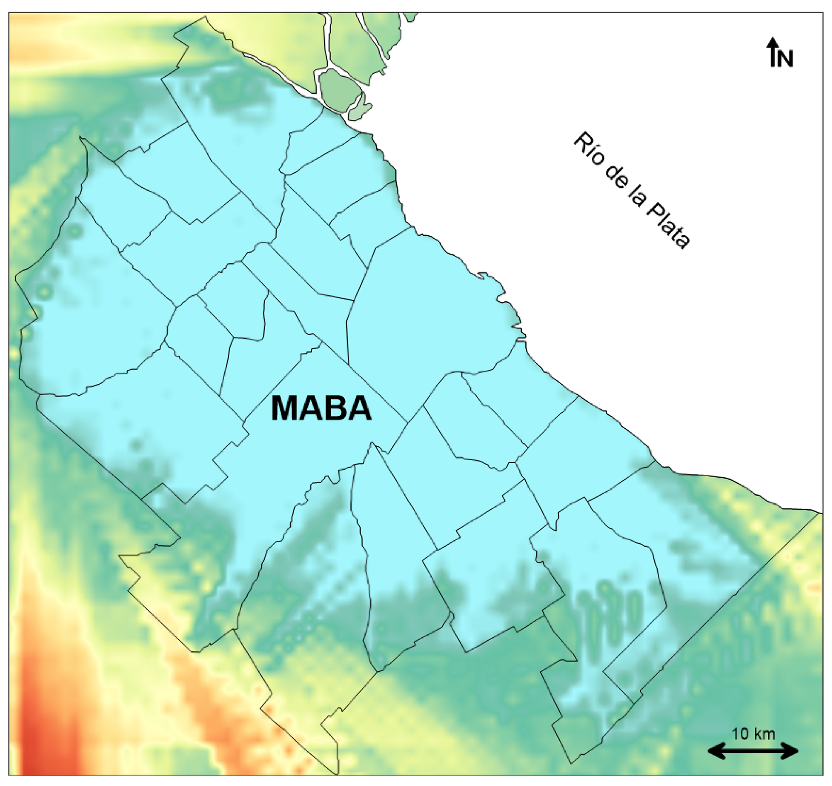
- ➢ An object is a set of conditions in which C_{max} occurs: its hour of occurrence and nine perturbed model input variables (M=10)
- ➢ Each variable is scaled subtracting its mean and dividing by its standard deviation across the whole modelling domain:

$$x' = \frac{x - \bar{x}}{\sigma_x}$$

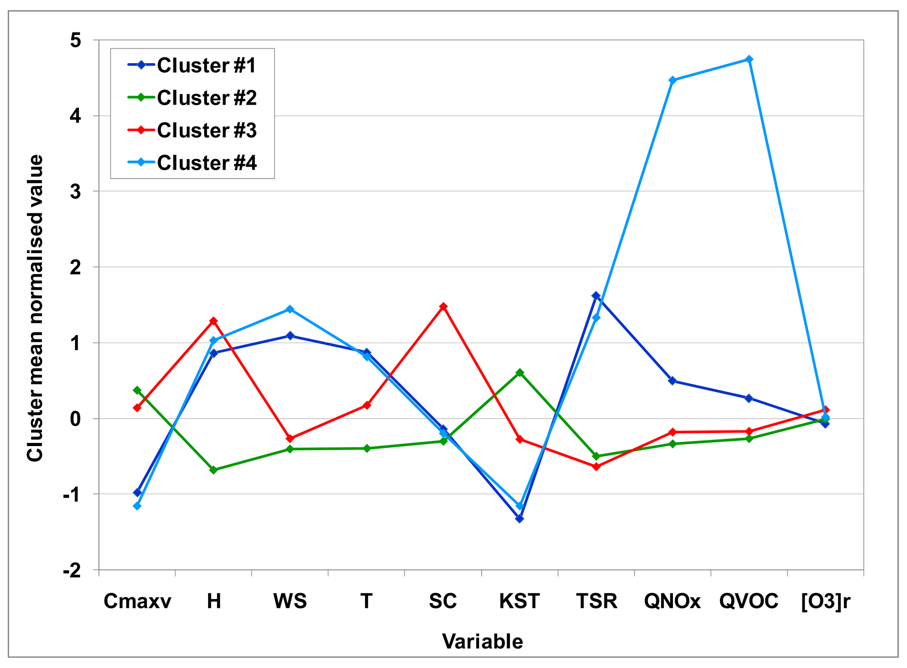
- ➢ The Matlab function kmeans is used with k=4, and 100 random initializations are performed to avoid suboptimal solutions

RESULTS AND CONCLUSIONS

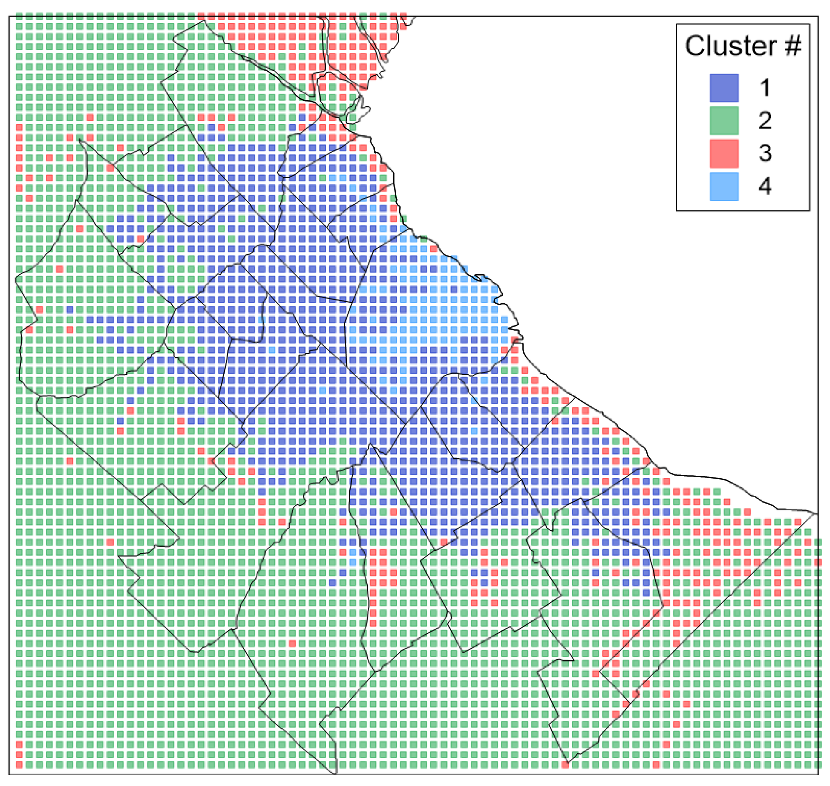
Probability of occurrence of values of C_{max} ≥ 40 ppb



Normalised variables (z-score) averaged for each cluster



Dominant cluster

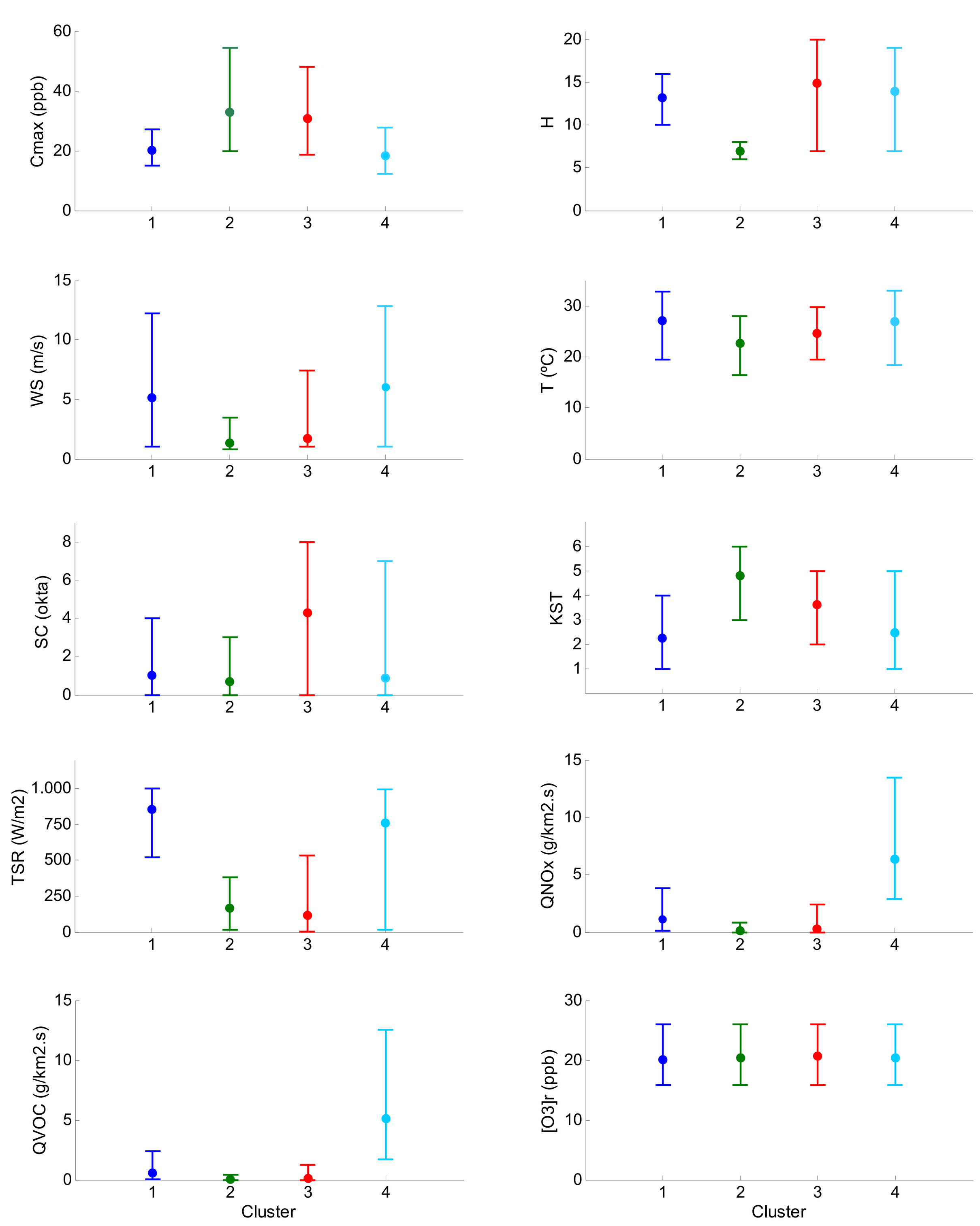


Variables averaged for each cluster

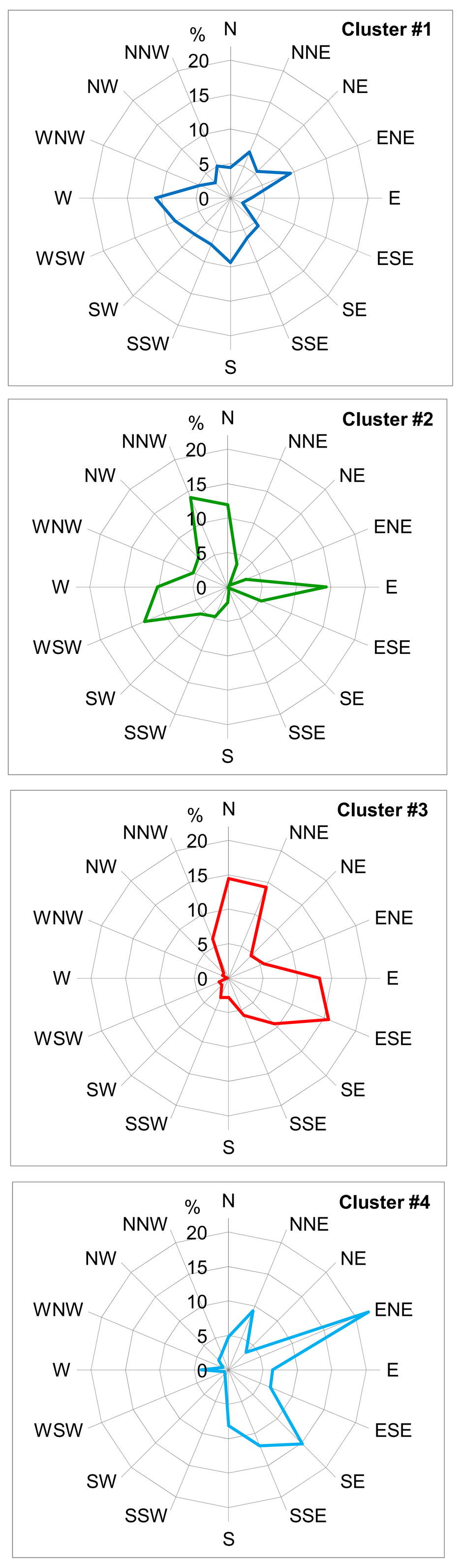
cluster #	C_{max} (ppb)	H	WS (m/s)	T (°C)	SC (okta)	KST	TSR (W/m^2)	QNOx (g/km^2s)	QVOC (g/km^2s)
1	20.2	13	5.1	27.0	1	2	854.9	1.2	0.6
2	32.9	7	1.3	22.4	1	5	166.5	0.1	0.0
3	30.8	15	1.7	24.5	4	4	119.8	0.3	0.1
4	18.5	14	6.0	26.8	1	2	762.3	6.3	5.1

C_{max}: summer maximum O_3 hourly concentration
H: hour of occurrence of C_{max}
WS: wind speed
T: air temperature
SC: sky cover
KST: atmospheric stability class
TSR: total solar radiation
QNO_x: local emission rate of NO_x
QVOC: local emission rate of VOCs
$[O_3]_r$: regional background O_3 concentration

Variables' mean and 95% confidence range vs cluster number



Wind roses of each cluster



CONCLUSIONS

✓ The probability of occurrence of values of C_{max} ≥ 40 ppb is very low in the urban area and greater than 70% outside the MABA

✓ From the clustering analysis, three main clusters with a marked spatial distribution resembling that of the O_3 precursor species emissions are obtained

✓ Differences in the mean variables of the clusters suggest different main drivers on ozone formation: photochemical (clusters 1, 3 and 4) vs dispersive (cluster 2)

REFERENCES

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[2] Pineda Rojas, A.L.; Venegas, L.E. 2013b. Spatial distribution of ground-level urban background O_3 concentrations in the Metropolitan Area of Buenos Aires, Argentina. *Environ. Pollut.*, 183, 159-165.

[3] Pineda Rojas, A.L., Venegas, L.E.; Mazzeo, N.A. 2016. Uncertainty of modelled urban peak O_3 concentrations and its sensitivity to input data perturbations based on the Monte Carlo analysis. *Atmos. Environ.*, 141, 422-429.

[4] Hanna, S.R.; Chang, J.C.; Fernau, M.E. 1998. Monte Carlo estimates of uncertainties in predictions by a photochemical grid model (UAM-IV) due to uncertainties in input variables. *Atmos. Environ.*, 32, 21, 3619-3628.