SENSITIVITY OF MODELLED URBAN BACKGROUND OZONE CONCENTRATIONS TO UNCERTAINTIES IN THE GRS INPUT VARIABLES

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MOTIVATION AND OBJECTIVES

The Generic Reaction Set (GRS) [1] is a simplified photochemical scheme which allows the estimation of ground-level O_3 concentrations at urban-scale and it is included in the algorithms of several air quality models (e.g., ADMS-Urban, TAPM, SOMS). Recently, the GRS was coupled with the DAUMOD model [2]. As part of the performance evaluation of the DAUMOD-GRS model in the Metropolitan Area of Buenos Aires (MABA), Argentina, in this work we explore the role that the variables representing an input for the GRS play on the modelled O_3 concentration uncertainty.

Objectives:

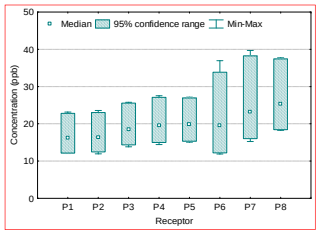
- To evaluate the uncertainty of the summer maximum O_3 diurnal peak 1 h-concentrations (C_{max}) modelled in the MABA with the DAUMOD-GRS due to uncertainties in the GRS input variables

- To analyse the sensitivity of the results to the magnitude of such uncertainties.

RESULTS

C_{max} uncertainty under conditions of Exp-2

Uncertainty of C_{max} at each selected receptor



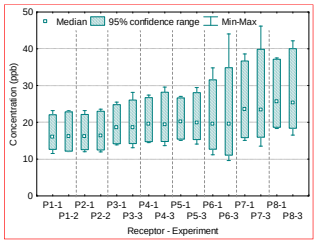
Uncertainty contribution of the GRS input variables to C_{max} uncertainty

Receptor	k's		C_iNO_x		C_iO_3	
	%	ppb	%	ppb	%	ppb
P1	3.1	0.3	4.7	0.5	72.7	7.7
P2	2.7	0.3	5.0	0.5	73.2	7.7
P3	0.5	0.1	1.2	0.1	84.7	9.5
P4	0.4	0.1	1.1	0.1	85.5	10.4
P5	0.2	<0.1	0.4	<0.1	88.5	10.2
P6	0.2	0.1	4.2	0.9	67.5	14.6
P7	0.2	<0.1	2.7	0.6	78.6	17.4
P8	<0.1	<0.1	0.2	<0.1	89.8	17.1

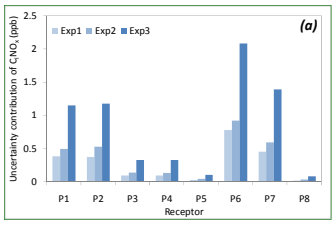
k's: sum of k_1 to k_4

Sensitivity of C_{max} uncertainty to the GRS input variables' uncertainties

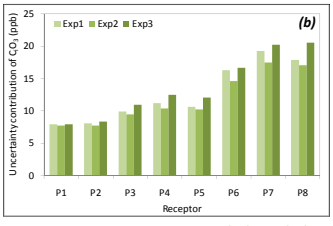
Uncertainty of C_{max} under conditions of the two Exp. presenting the greatest difference



Contributions of C_iNO_x (a) and C_iO_3 (b) to C_{max} uncertainty under conditions of experiments 1, 2 and 3



Maximum-to-minimum ratio: 2.7 (P6) – 3.8 (P8)



Maximum-to-minimum ratio: 1.0 (P1) - 1.2 (P4)

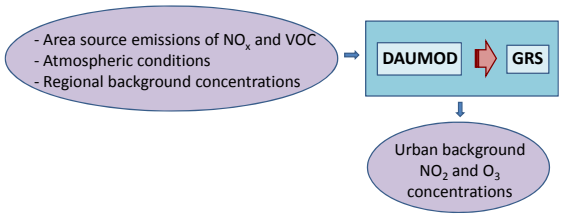
➢ The greatest C_{max} uncertainty is obtained under conditions of Exp-3 at all receptors

➢ An increase of C_iNO_x uncertainty of a factor of 2.7 (from 30% to 80%) leads to an increase of its contribution to C_{max} uncertainty that varies between 2.7 and 3.8 among selected receptors

REFERENCES
[1] Azzi, M., Johnson, G., Cope, M., 1992. An introduction to the generic reaction set photochemical smog model. In: Proc. 11th Int. Clean Air Conf., pp. 451-462.
[2] Pineda Rojas, A.L.; Venegas, L.E. 2013a. Upgrade of the DAUMOD atmospheric dispersion model to estimate urban background NO_2 concentrations. *Atmos. Res.*, **120-121**, 147-154.
[3] 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.
[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.

METHODOLOGY

The DAUMOD-GRS model [2]



Zero-uncertainty (ZU) run conditions

- Surface hourly meteorological data measured at the domestic airport (summer 2007)
- Sounding data from the station located at the international airport
- High-resolution (1km^2, 1h) area source emissions of NO_x and VOC for the MABA
- Clean air regional background concentrations for all species

✓ The performance of the DAUMOD-GRS to simulate peak O_3 concentrations at sixteen monitoring sites in the MABA under such conditions is discussed in [3].

Evaluation of C_{max} uncertainty

Monte Carlo (MC) analysis: a large number of simulations (N) is performed considering alternative values of the **GRS input variables**, within their possible ranges of error. This leads to N probable results of C_{max} from which its uncertainty is estimated.

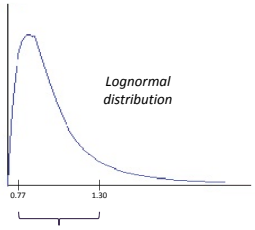
- Reaction constant rates (k_1-k_4)
- Initial concentrations (C_iNO_x, C_iVOC, C_iO_3)

Since errors in such model internal variables are not really known, three different combinations are considered:

Considered errors for the GRS input variables in each experiment

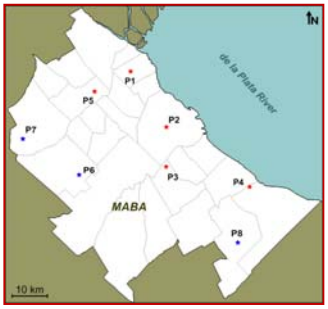
Variable	Exp-1	Exp-2	Exp-3
k_1-k_4	30%	30%	30%
C_iNO_x	30%	50%	80%
C_iVOC	30%	50%	80%
C_iO_3	30%	30%	40%

Commonly found in the literature, e.g. [4]



N=100 perturbation values are obtained for each variable and experiment, using Simple Random Sampling

Selected receptors at the Metropolitan Area of Buenos Aires (MABA), Argentina. The hour of occurrence of C_{max}(ZU) is highlighted [red: 11-14h, blue: 7-8h or 19h]



The MC runs are performed for eight selected receptors presenting a wide range of atmospheric and emission conditions which are associated to the varying time (day of summer and hour) of occurrence of C_{max}(ZU)

Multiple Linear Regression Analysis (MLRA) is then applied to assess the relative contribution from each variable to the estimated C_{max} uncertainty.

CONCLUSIONS

✓ Uncertainty of C_{max} varies spatially, being greater at receptors where O_3 peaks occur in the early morning or late evening than where C_{max} occurs around midday hours.

✓ The relative contributions from the uncertainties in the GRS input variables vary spatially, although that of C_iO_3 dominates at all analysed receptors.

✓ The sensitivity of C_{max} uncertainty to the input variables' uncertainty varies among the selected receptors between 1.0 ppb (10%) and 5.0 ppb (26%). The relative contribution of C_iNO_x is more sensitive to its uncertainty than that of C_iO_3.