



ITM 2026



**Barcelona
Supercomputing
Center**
Centro Nacional de Supercomputación



AI4S
BSC AI 4 Science Fellowships

Impact of chemical mechanism complexity on modelled ozone formation potential and ~~secondary organic aerosol potential~~ in the Barcelona plume.

Camille Mouchel-Vallon, Hervé Petetin, Oriol Jorba Casellas, Kevin Oliveira, and Marc Guevara

Impact of emission change in a chemistry transport model

Example: *Effect of different emission inventories on modeled ozone and carbon monoxide in Southeast Asia (Amnuaylojaroen et al., 2014)*

RETRO

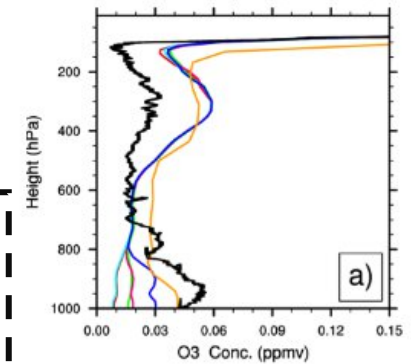
INTEX-B

MACCITY

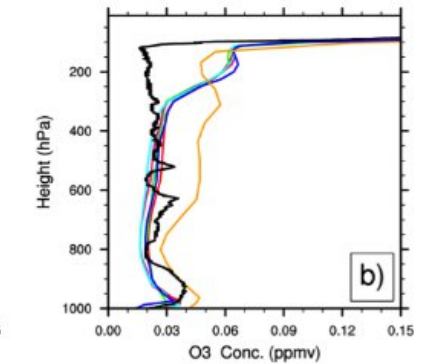
SEAC4RS

WRF-Chem

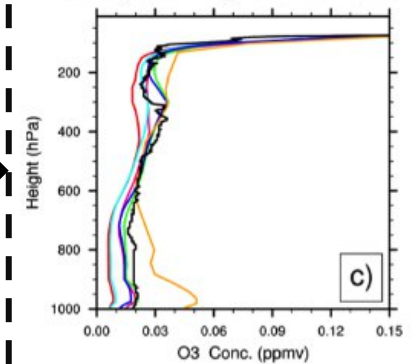
Watukosek Java, O₃ Mixing Ratio, March 13, 2008



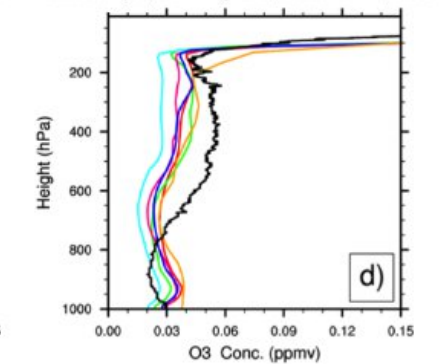
Watukosek Java, O₃ Mixing Ratio, December 11, 2008



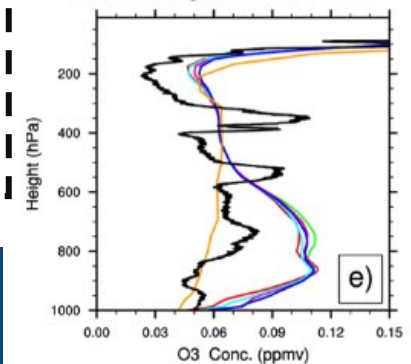
Kuala Lumpur, O₃ Mixing Ratio, March 17, 2008



Kuala Lumpur, O₃ Mixing Ratio, December 17, 2008



Hanoi, O₃ Mixing Ratio, March 12, 2008



How does an emission change become an O₃ change?

What is really happening (in the model) to emitted VOC?

How does the choice of the chemical mechanism affect the sensitivity of modeled pollutants to VOC emissions?

WRF-Chem: MOZART, CAM-Chem
CHIMERE: MELCHIOR, SAPRC-07A
CMAQ: CB05, CB6, CRACMM1, CRACMM2, RACM2, SAPRC07

Emission Inventory Species

CO,
NO_x,
SO₂,
NH₃,
...
NMVOC

VOCs
aggregation/disaggregation

Chemistry Transport Model (simplified)

chemical
mechanism

ODEs
integration

O₃
concentration

Many reasons to be aware of modeled pollutants **sensitivity to emitted VOCs**: update to inventory, inclusion of new VOCs, future scenarios, impact of pollution mitigation policy, air quality directive...

The chemical mechanism selection also controls the **aggregation/disaggregation** of Inventory Species to Model Species

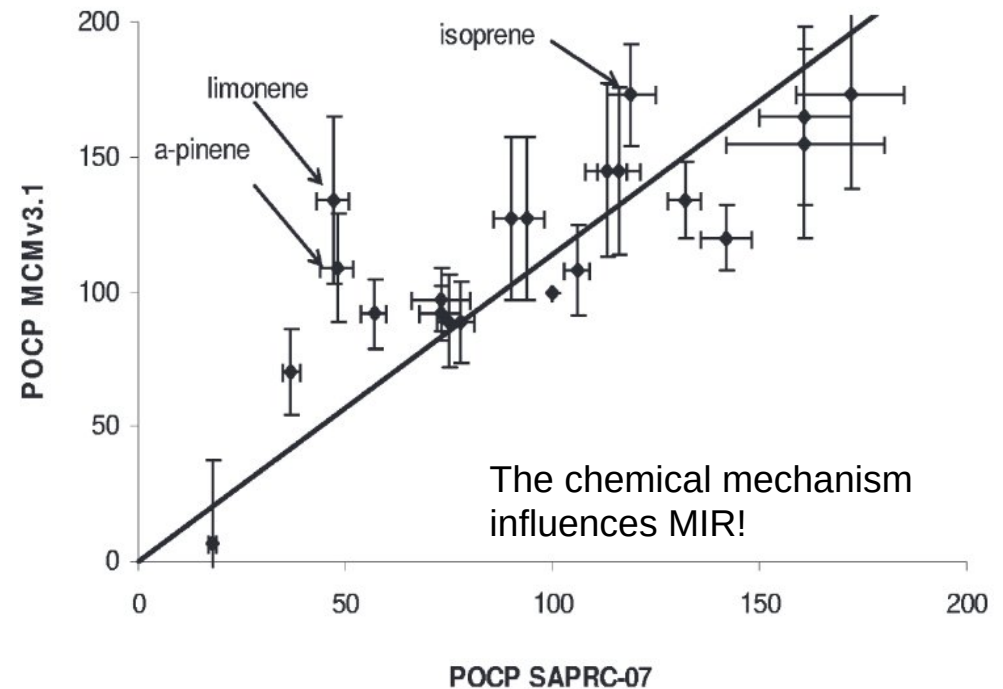
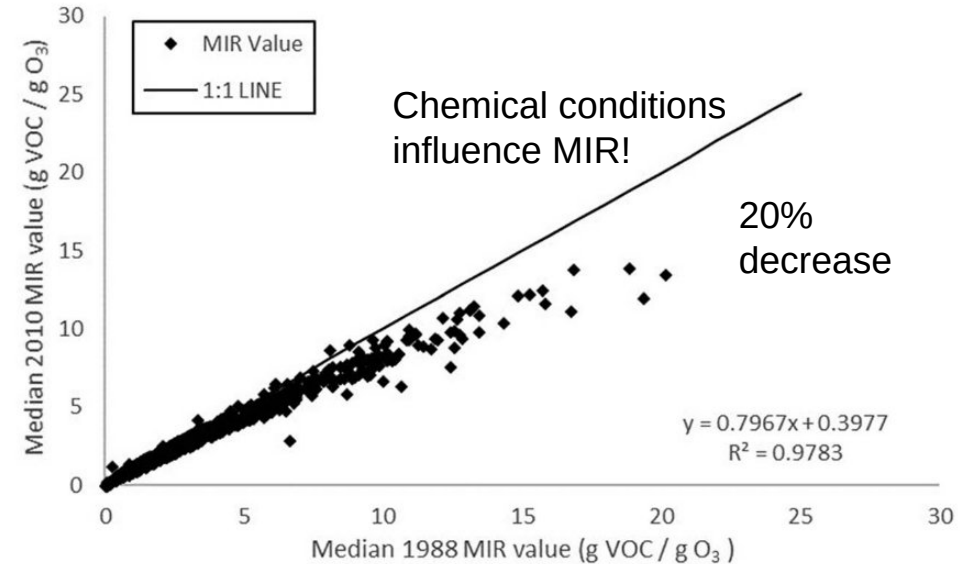
The CTM is estimating the impact on air quality through the lens of the **selected chemical mechanism**

Measuring ozone sensitivity to VOC emission change

The Maximum Increased Reactivity scale (Carter, 1994a, 2010, Venecek et al., 2018, ...)

- Ideal boxmodel simulations of 1988 urban areas pollution plumes
 - NO_x emissions selected for highest O₃ sensitivity to VOC
 - In turn, increase each VOC emission by a small amount
 - MIR: change in max(O₃) per unit of added VOC
-
- systematically calculated for 39 cities across the USA
 - updated for each version of SAPRC90 to SAPRC07
 - updated scenario to 2010 conditions in Venecek et al., 2018
-
- Derwent et al. (2010) comparison SAPRC vs MCM3.1

Detailed models are rarely used in real air quality studies



MIR for a simplified chemical mechanism

Carter (1994b): Compute MIR directly for Carbon Bond 4 model species

- Use emission aggregation tables to calculate MIR of explicit VOCs, assuming that MIR can be combined linearly

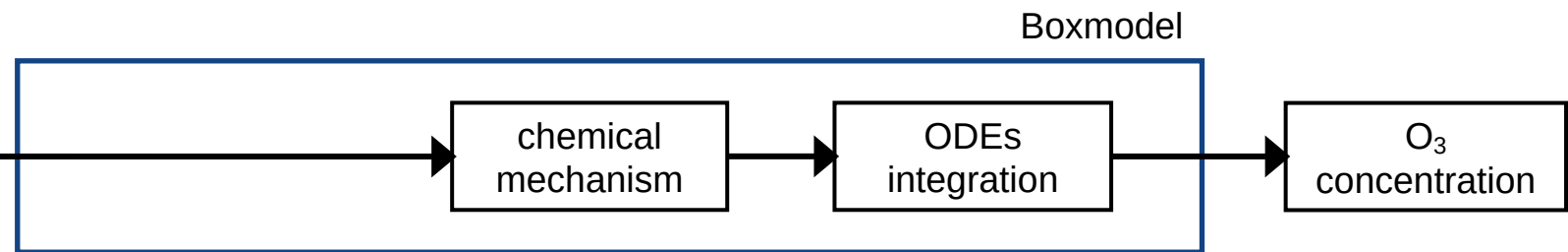
Table 10. Incremental Reactivities for Carbon Bond model species and the ba ROG mixture in the individual Maximum Reactivity scenarios. Units a mol O₃/mol

Scen.	CO	PAR	ETH	OLE	TOL	XYL	HCHO	ALD2	ISOP	MEOH	ETOH	MTBE	B.ROG
ATL GA	0.0270	0.308	4.39	8.89	3.10	16.87	5.06	5.38	19.77	0.390	1.239	1.064	0.882
AUS TX	0.0300	0.363	4.54	9.53	3.25	17.87	5.26	5.83	20.93	0.399	1.371	1.153	0.958
BAL MD	0.0330	0.358	4.99	10.37	4.54	21.59	6.38	6.88	23.58	0.420	1.415	1.406	1.046
BAT LA	0.0230	0.236	4.05	7.93	2.96	16.09	5.25	4.41	18.33	0.357	1.001	0.944	0.786
BIR AL	0.0350	0.468	5.51	11.67	4.47	22.97	6.71	7.59	26.08	0.496	1.729	1.370	1.224
BOS MA	0.0320	0.388	4.21	8.52	3.13	15.65	4.49	5.37	18.79	0.388	1.332	1.197	0.894
CHA NC	0.0330	0.432	4.32	8.59	3.14	15.40	4.01	5.53	18.24	0.407	1.502	1.246	0.916
CHI IL	0.0270	0.312	4.65	9.56	4.01	20.46	5.95	5.81	21.83	0.408	1.240	1.090	0.989
CIN OH	0.0350	0.418	4.93	10.50	3.93	20.40	5.83	6.86	23.58	0.431	1.531	1.373	1.075
CLE OH	0.0240	0.272	4.05	8.71	2.74	16.61	5.32	5.38	19.90	0.347	1.023	0.965	0.848
DAL TX	0.0250	0.292	4.12	8.74	2.90	16.80	5.38	5.08	19.76	0.361	1.152	1.001	0.860
DEN CO	0.0210	0.211	4.01	8.48	2.73	16.96	5.86	5.16	20.10	0.333	0.881	0.877	0.816
DET MI	0.0310	0.389	4.66	10.20	3.63	19.82	5.89	6.57	23.12	0.410	1.399	1.192	1.047
ELP TX	0.0210	0.213	4.14	8.96	2.75	17.72	5.87	5.32	20.71	0.338	0.952	0.875	0.842
HAR CT	0.0350	0.447	5.19	10.90	3.98	20.60	5.89	7.10	23.99	0.461	1.650	1.342	1.130
HOU TX	0.0360	0.391	5.07	10.33	4.58	21.47	6.17	6.42	23.50	0.451	1.519	1.446	1.065
IND IN	0.0300	0.344	4.98	10.56	3.65	20.80	6.52	6.54	24.01	0.435	1.365	1.172	1.055
JAC FL	0.0310	0.333	5.02	9.81	3.80	19.59	5.83	5.88	22.40	0.453	1.383	1.211	0.995
KAN MO	0.0350	0.460	5.27	11.12	4.03	20.98	5.95	7.20	24.39	0.468	1.714	1.349	1.152
TXV TX	0.0260	0.282	4.57	10.40	4.65	22.20	6.61	6.02	22.02	0.525	1.562	1.402	1.116

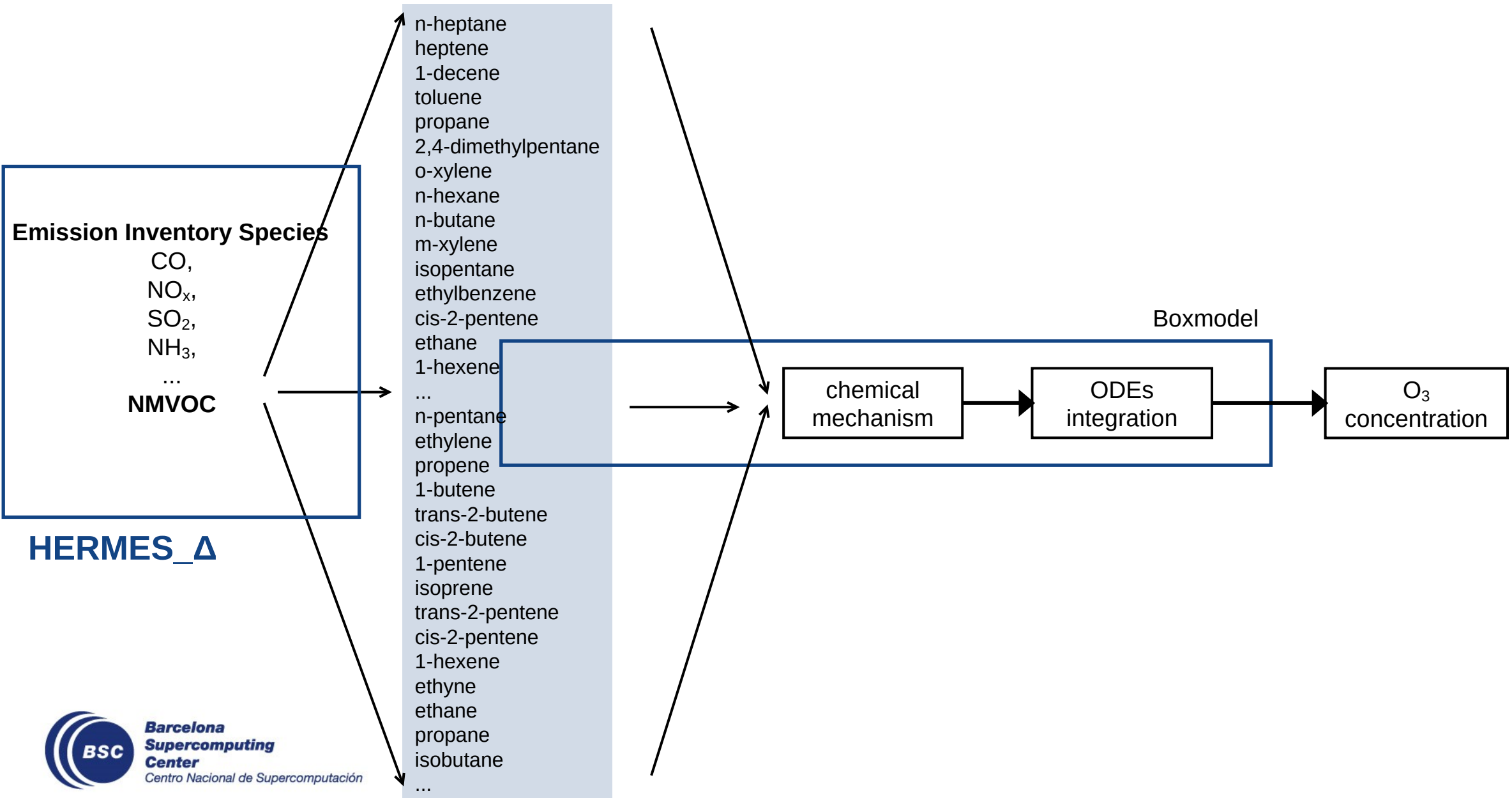
A tentative methodology to evaluate ozone sensitivity to chemical mechanisms choice

Emission Inventory Species

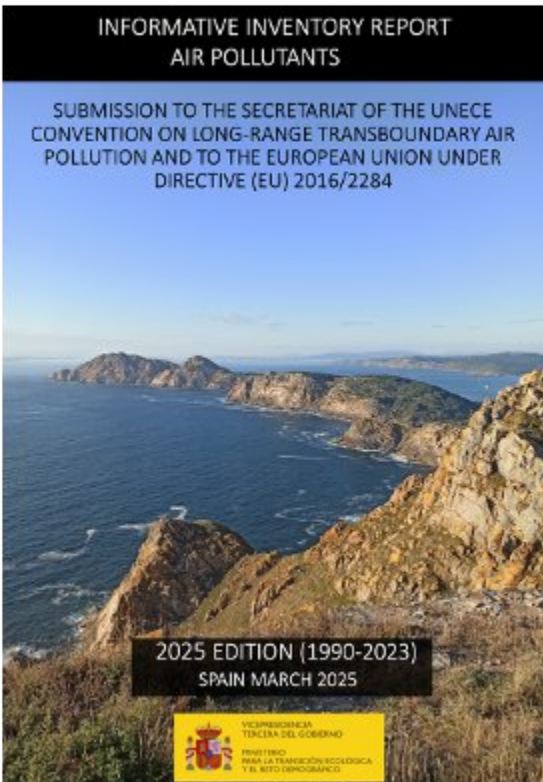
CO,
NO_x,
SO₂,
NH₃,
...
NMVOC



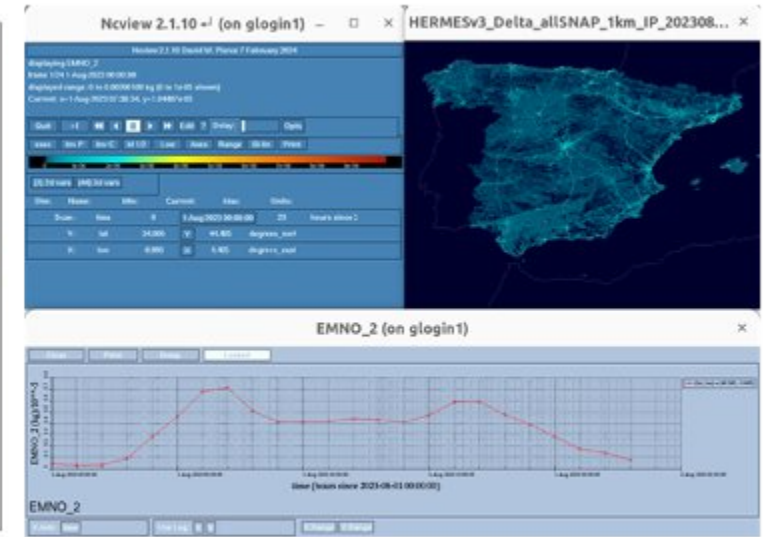
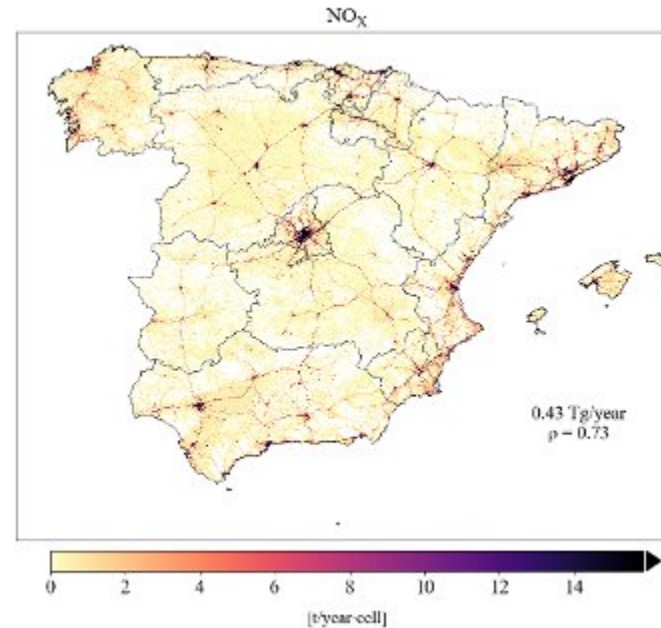
A tentative methodology to evaluate ozone sensitivity to chemical mechanisms choice



HERMES_Δ: A bottom up inventory for Spain

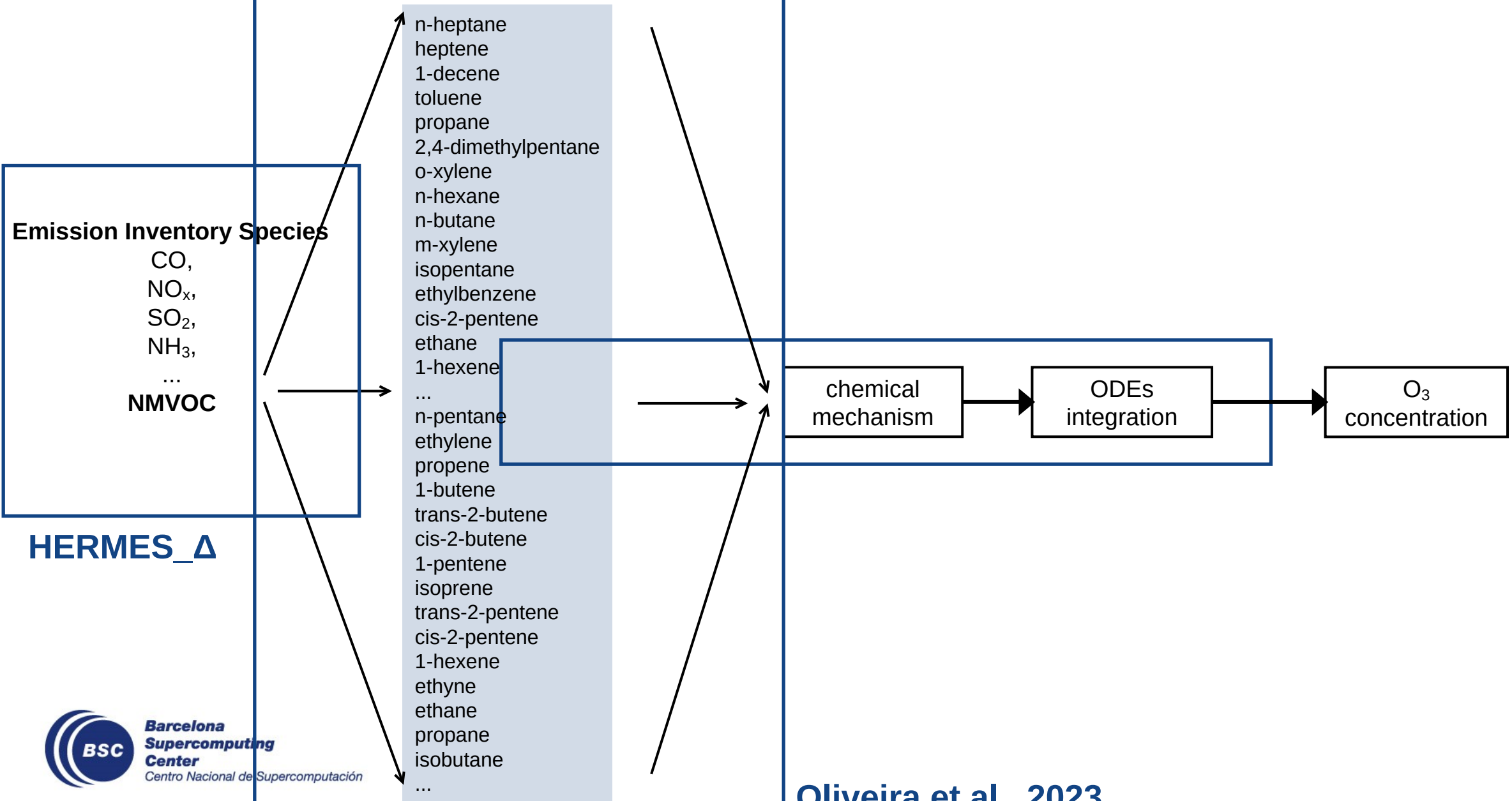


HERMES_Δ



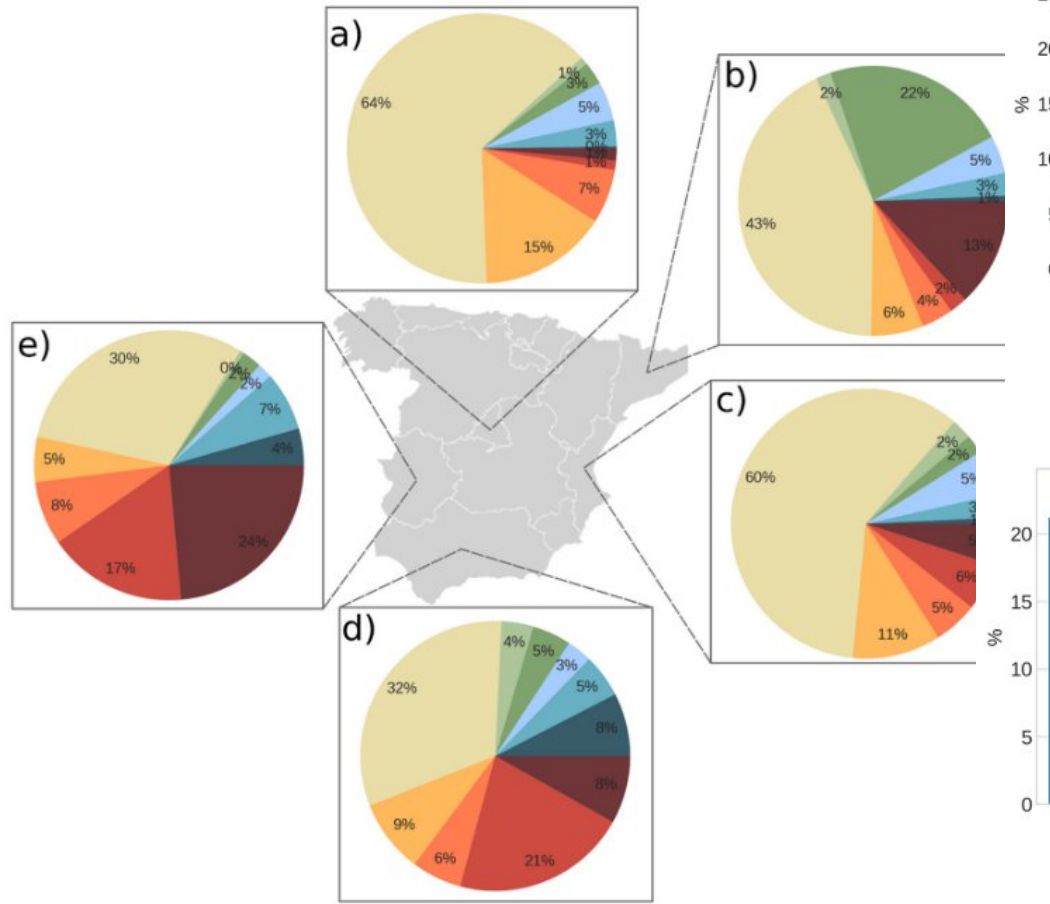
Spatial mapping of nationally reported emissions over a detailed map of pollution sources + Temporal hourly distribution by activity sector

A tentative methodology to evaluate ozone sensitivity to chemical mechanisms choice



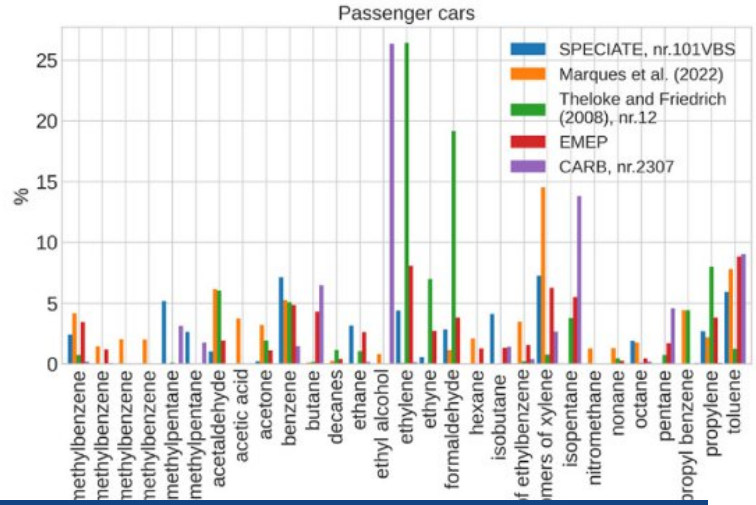
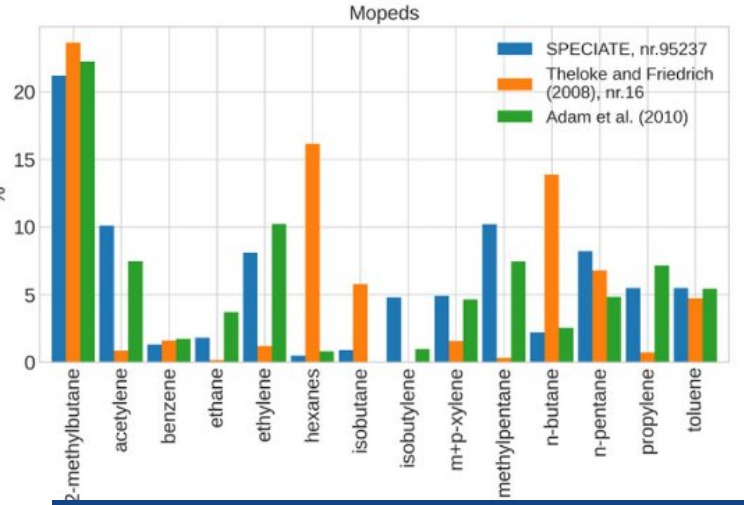
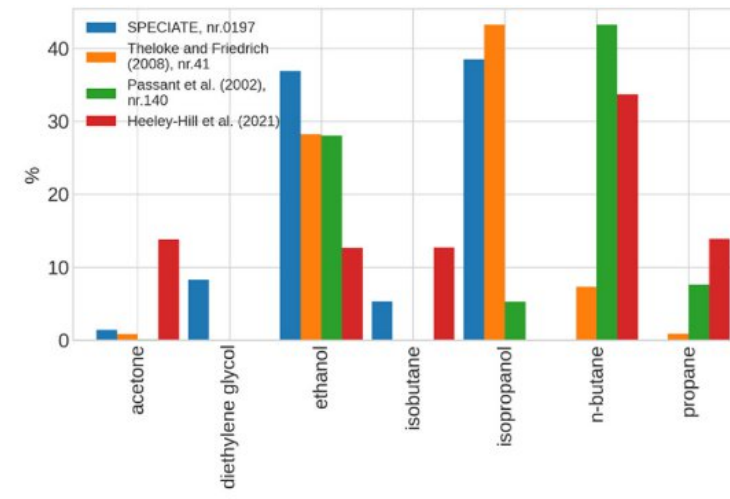
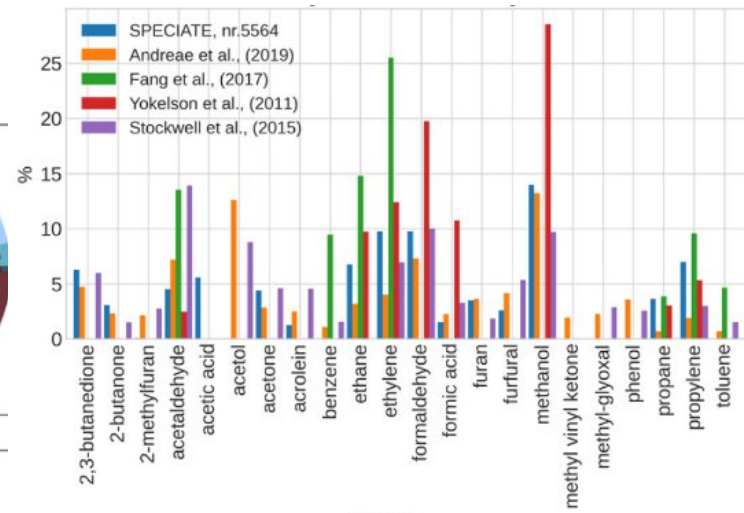
Oliveira et al., 2023: A detailed VOC speciation for HERMES_Δ

Disaggregation of VOCs into ~900 explicit species, according to emission sector, fuel source, factory types, etc...



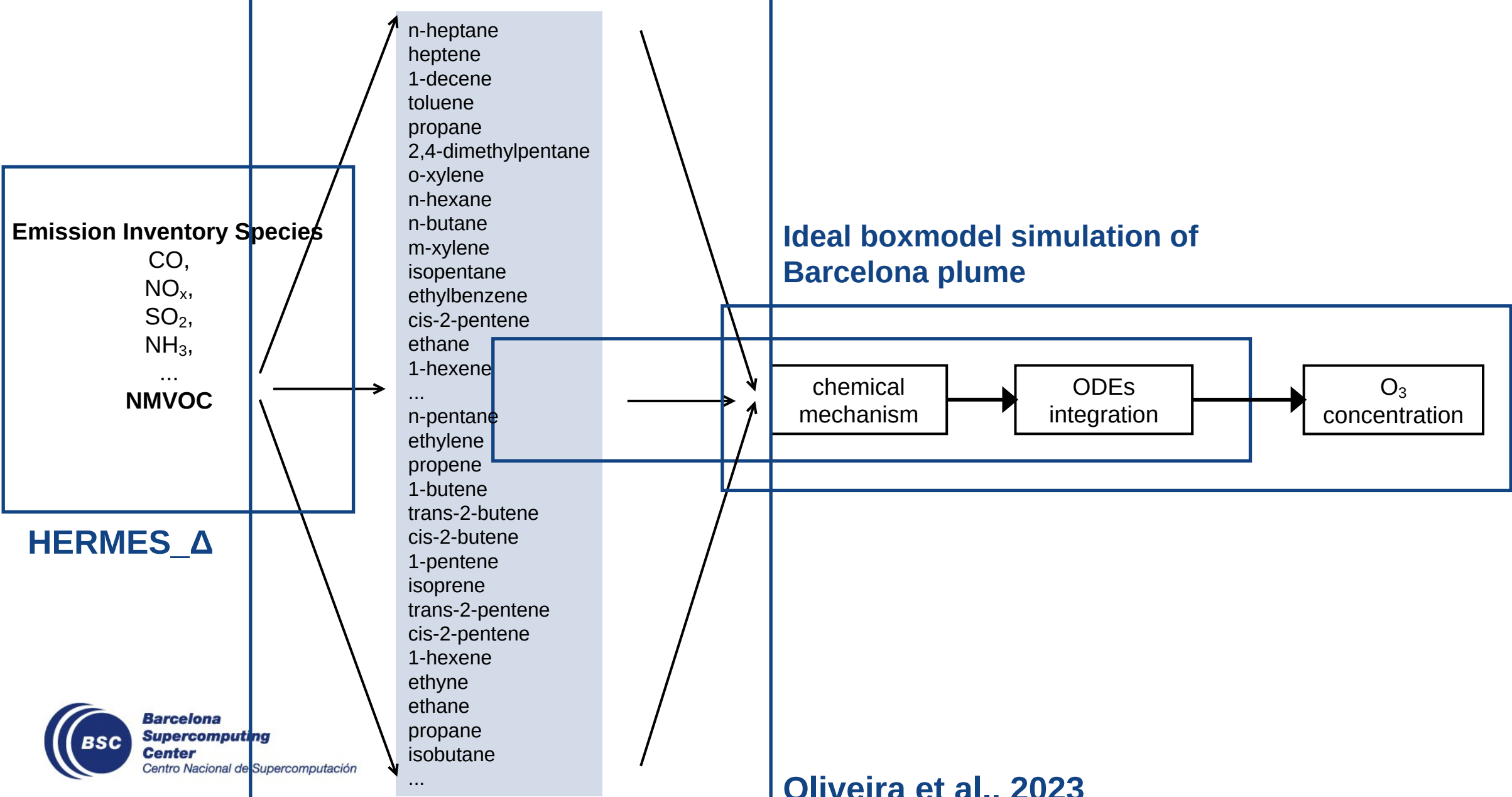
SNAP

- 01 - Combustion in energy and transformation industries
- 02 - Non-industrial combustion plants
- 03 - Combustion in manufacturing industry
- 04 - Production processes
- 05 - Extraction and distribution of fossil fuels
- 06 - Solvent and other product use
- 07 - Road transport
- 08 - Other mobile sources and non-road transport
- 09 - Waste collection, treatment and disposal
- 10 - Agriculture and farming



Available aggregation to multiple chemical mechanisms: CB05, CB6, RACM2, CRACMM1, CRACMM2, MELCHIOR, ...

A tentative methodology to evaluate ozone sensitivity to chemical mechanisms choice



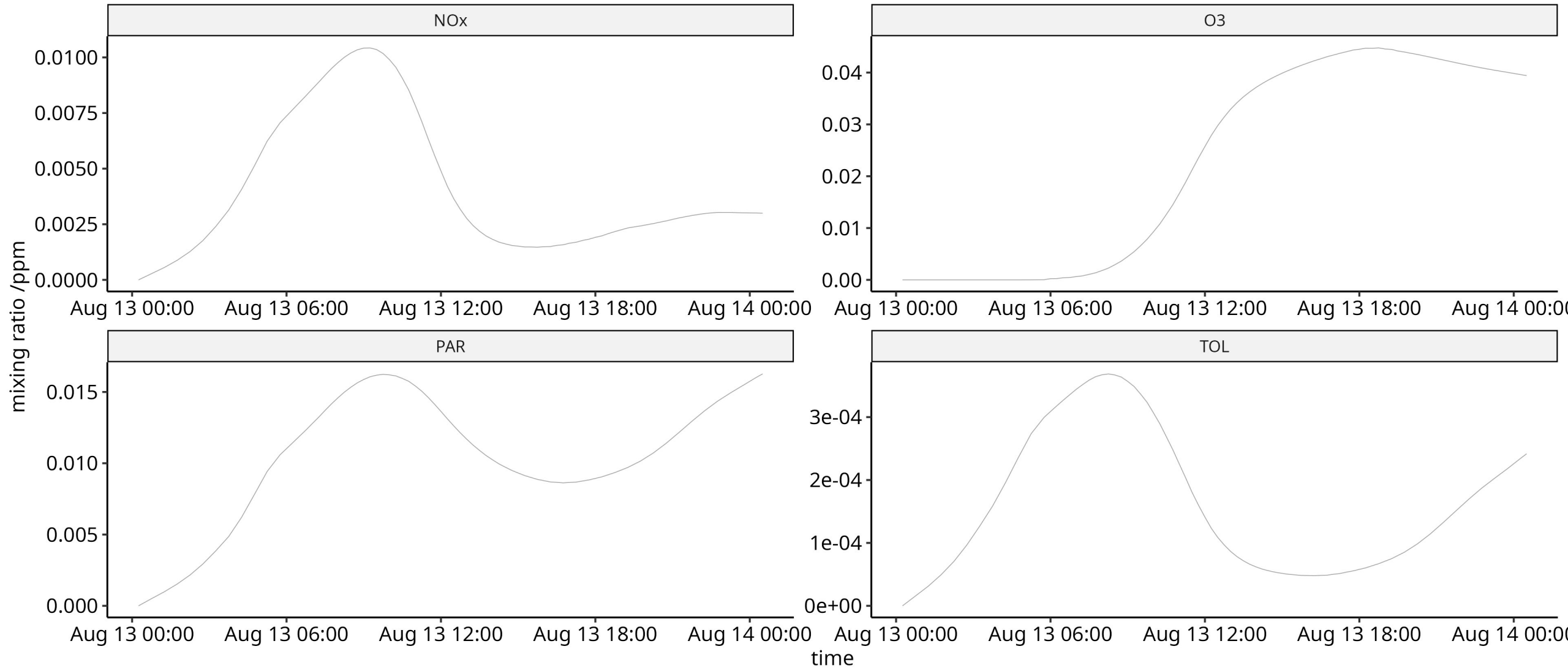
HERMES_Δ

Idealized boxmodel simulation in Barcelona

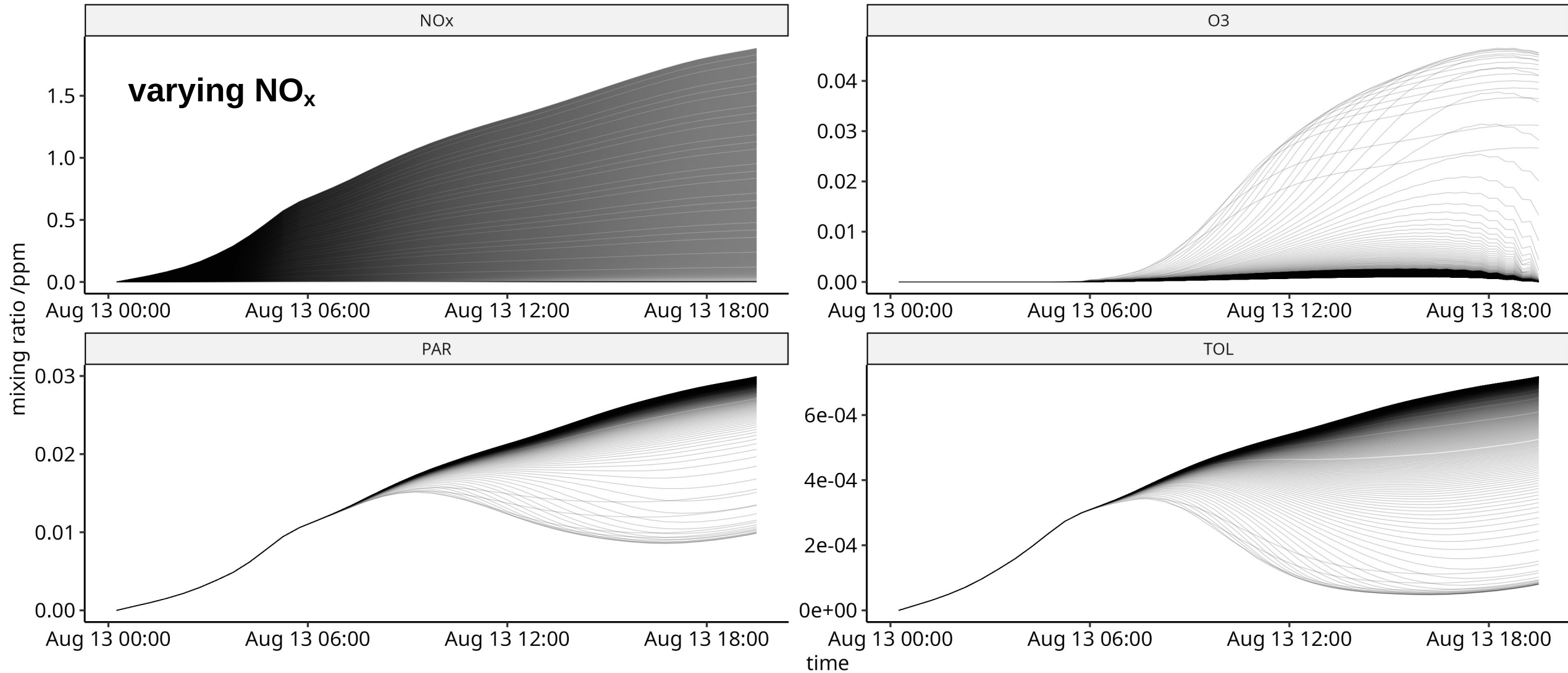


- Summer 2023 typical day
- HERMES_Δ emissions averaged over Barcelona
- NMVOC emissions speciation according to Oliveira et al. (2023)
- meteocat meteorological variables
- PBL height from MPLnet (lidar)
- Boundary conditions (dilution) from MONARCH

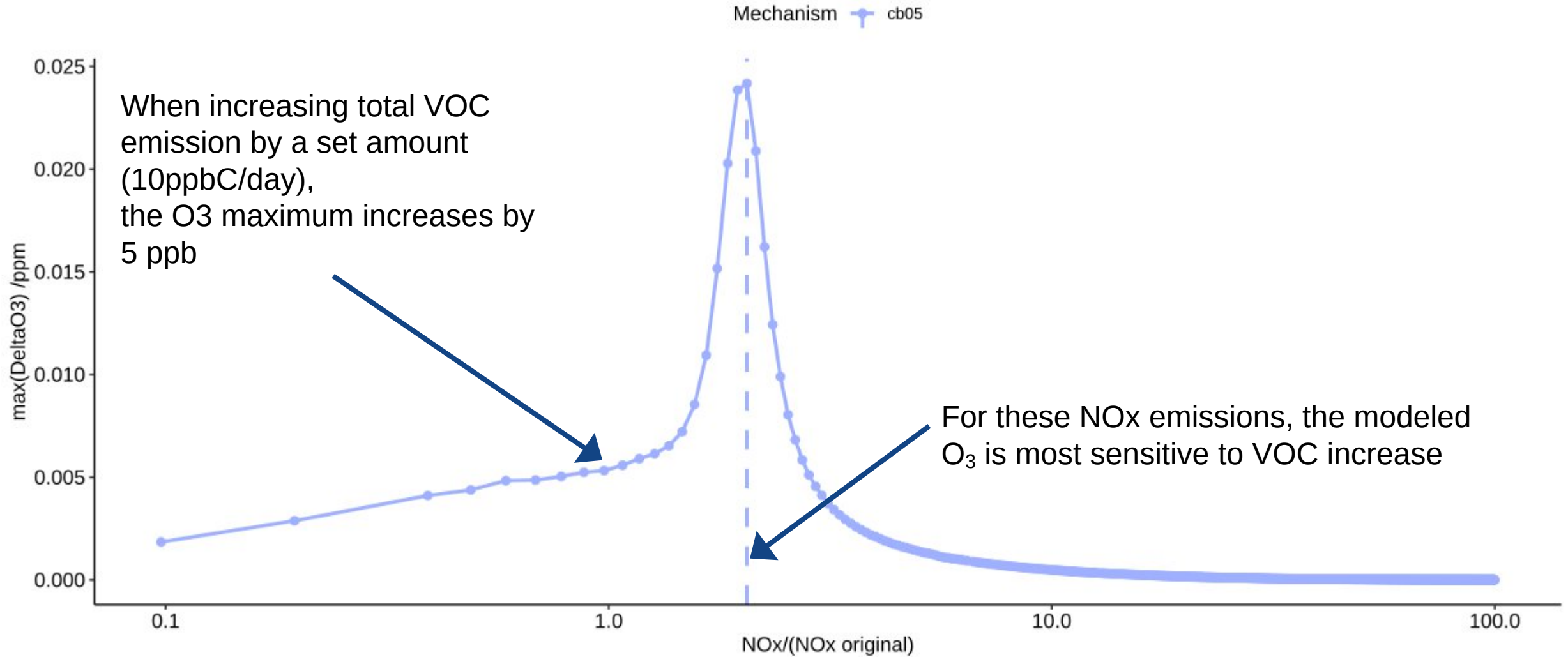
Barcelona: CB05 example



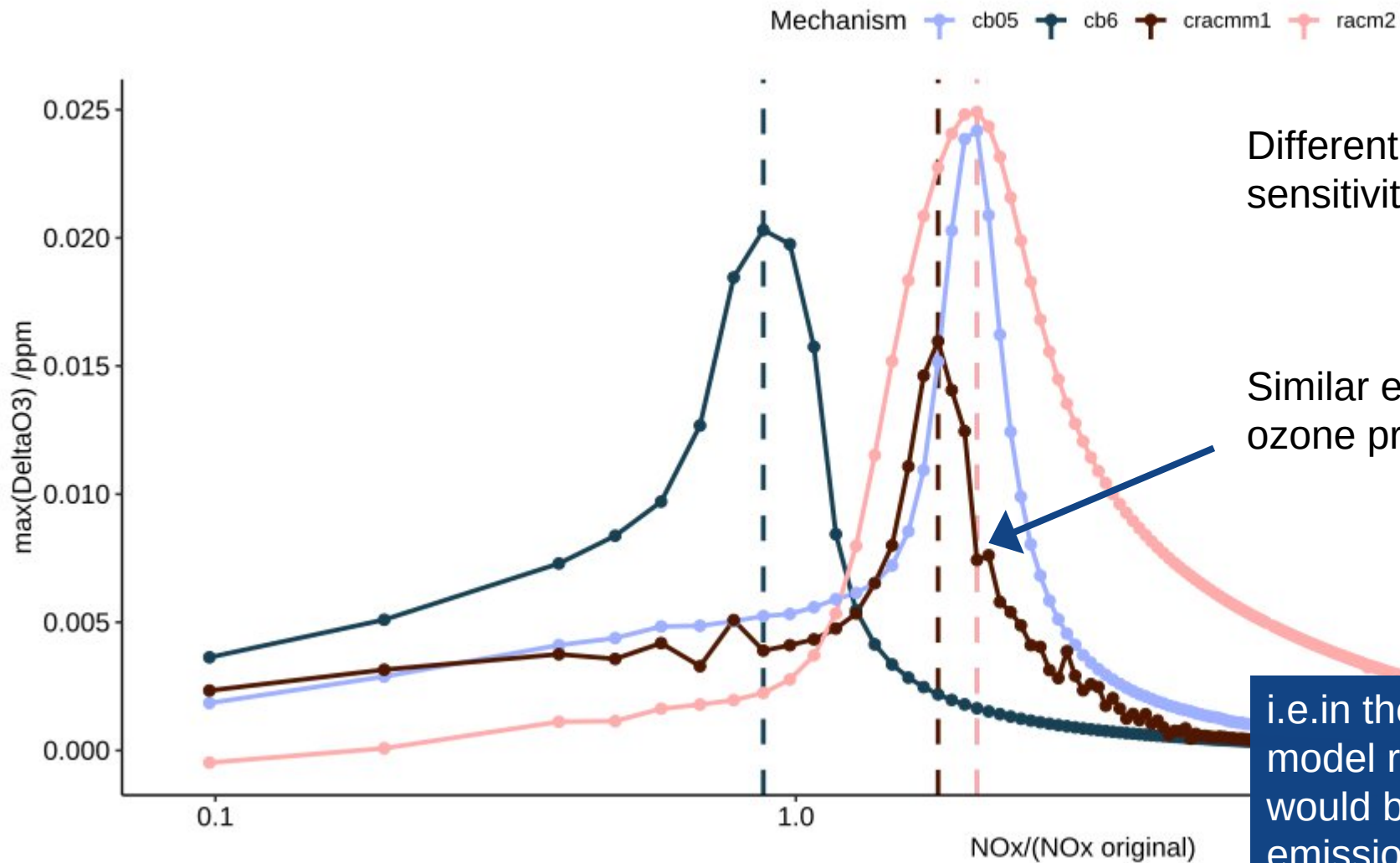
Barcelona: CB05 example



Barcelona: CB05 example



Barcelona: comparison with CB6, CRACMM1, RACM2



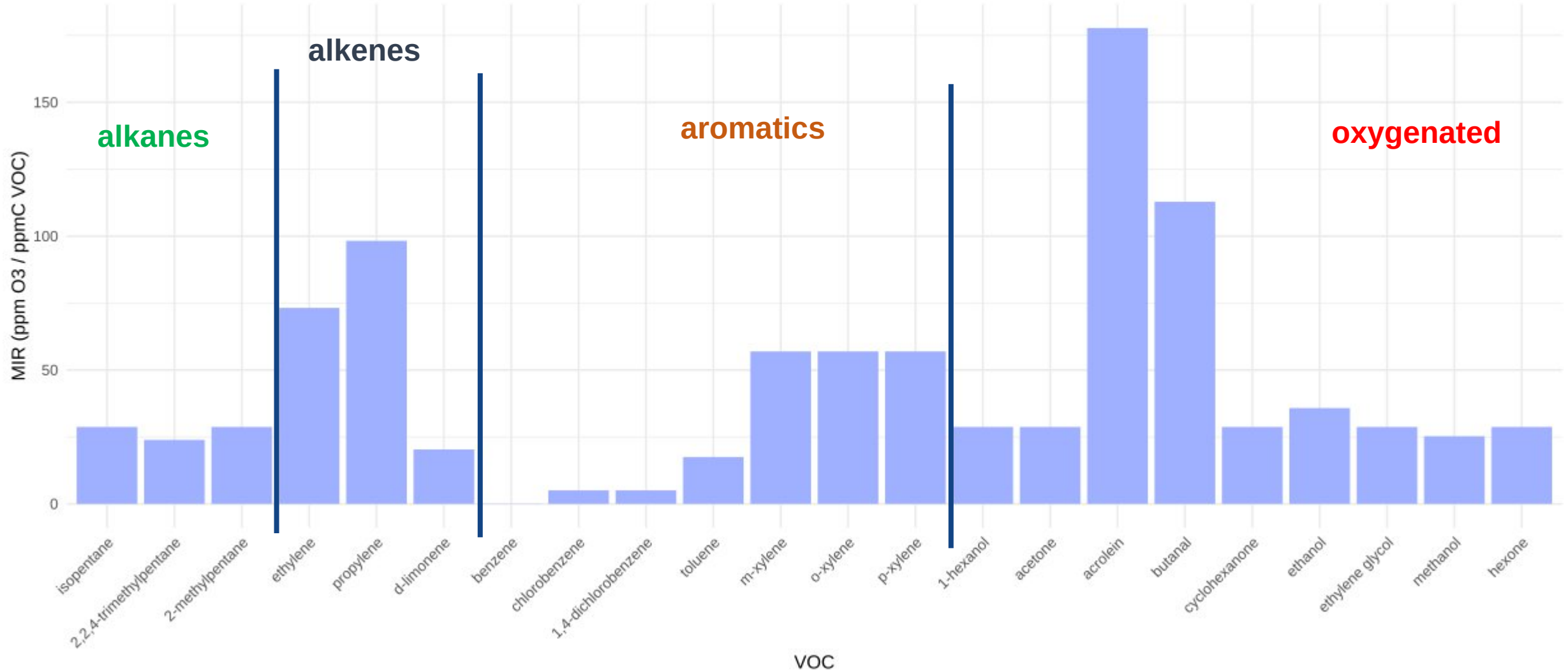
Different mechanism exhibit different sensitivities to NO_x emissions



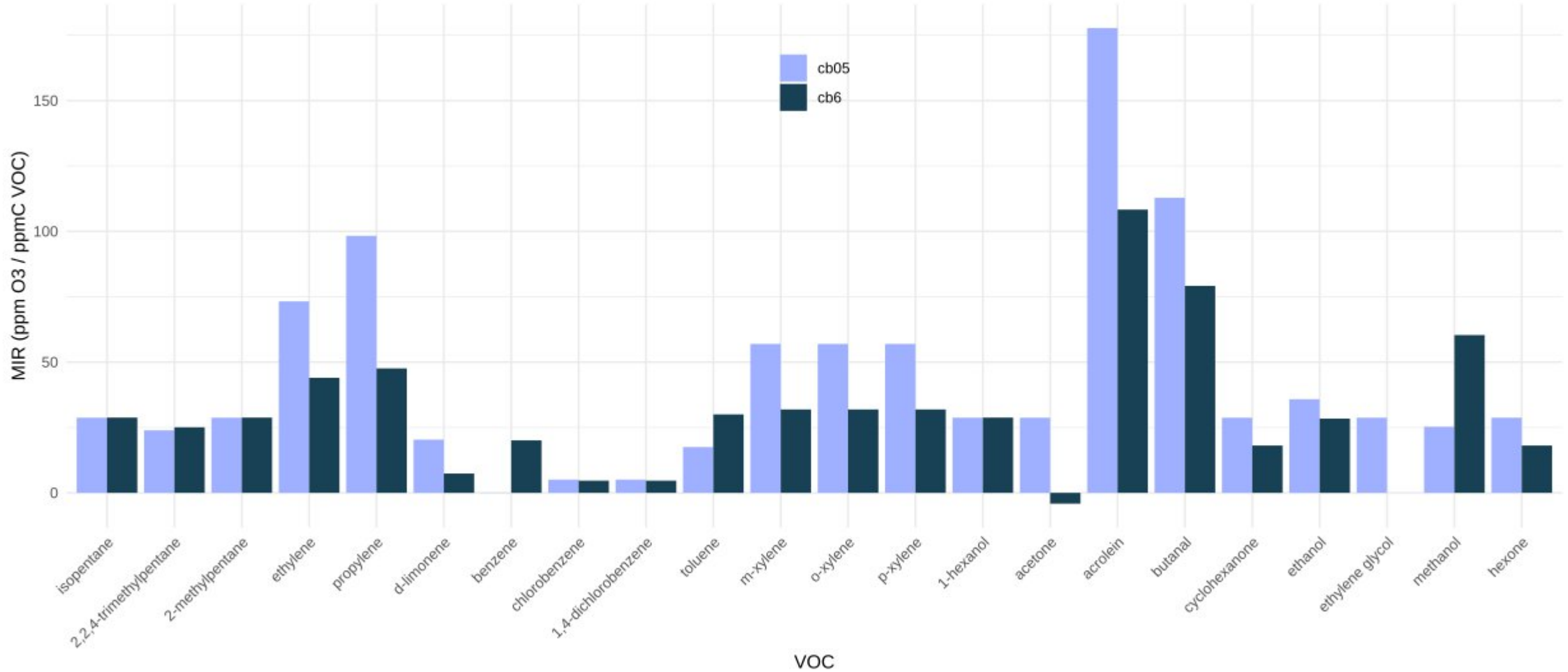
Similar emissions could yield different ozone production regimes

i.e. in the same chemical environment, a model running with RACM2 or CB05 would be more sensitive to VOC emission change than a model running with CRACMM1

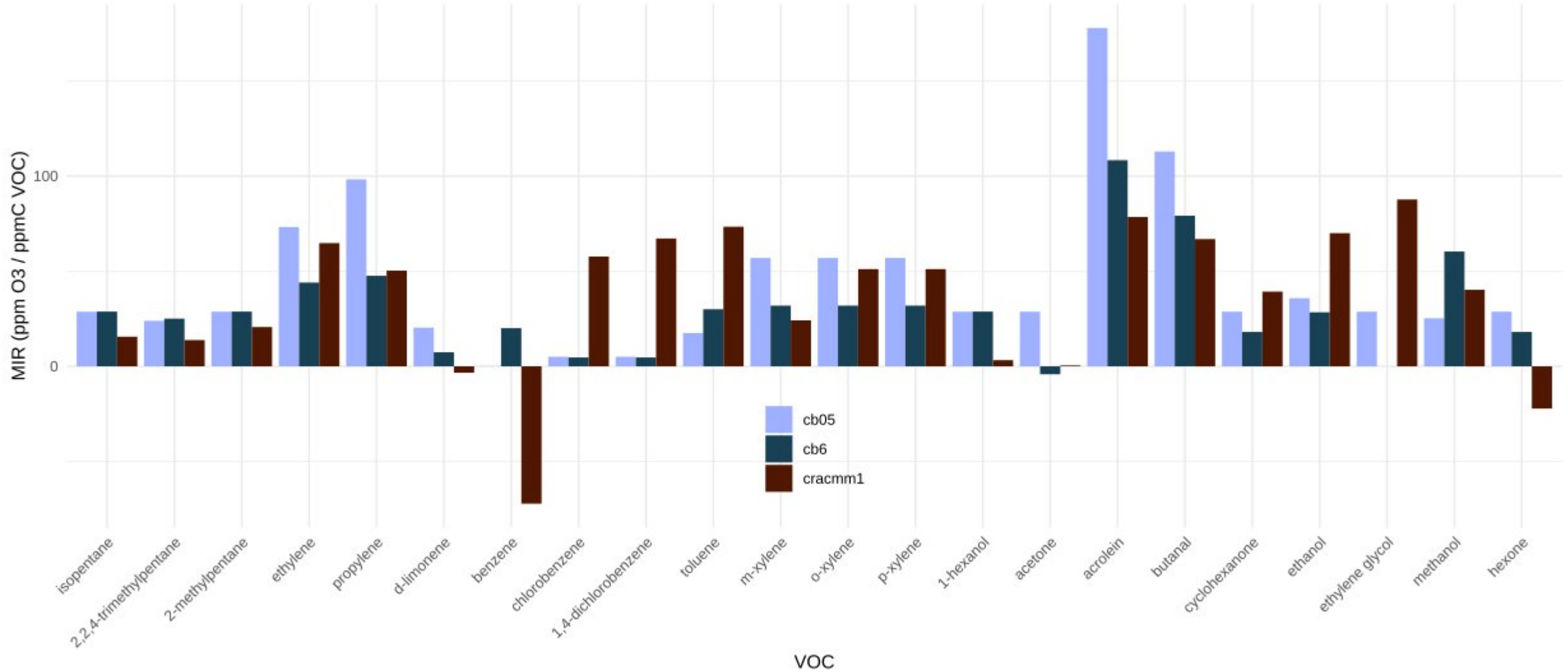
MIR in Barcelona: individual VOCs with CB05



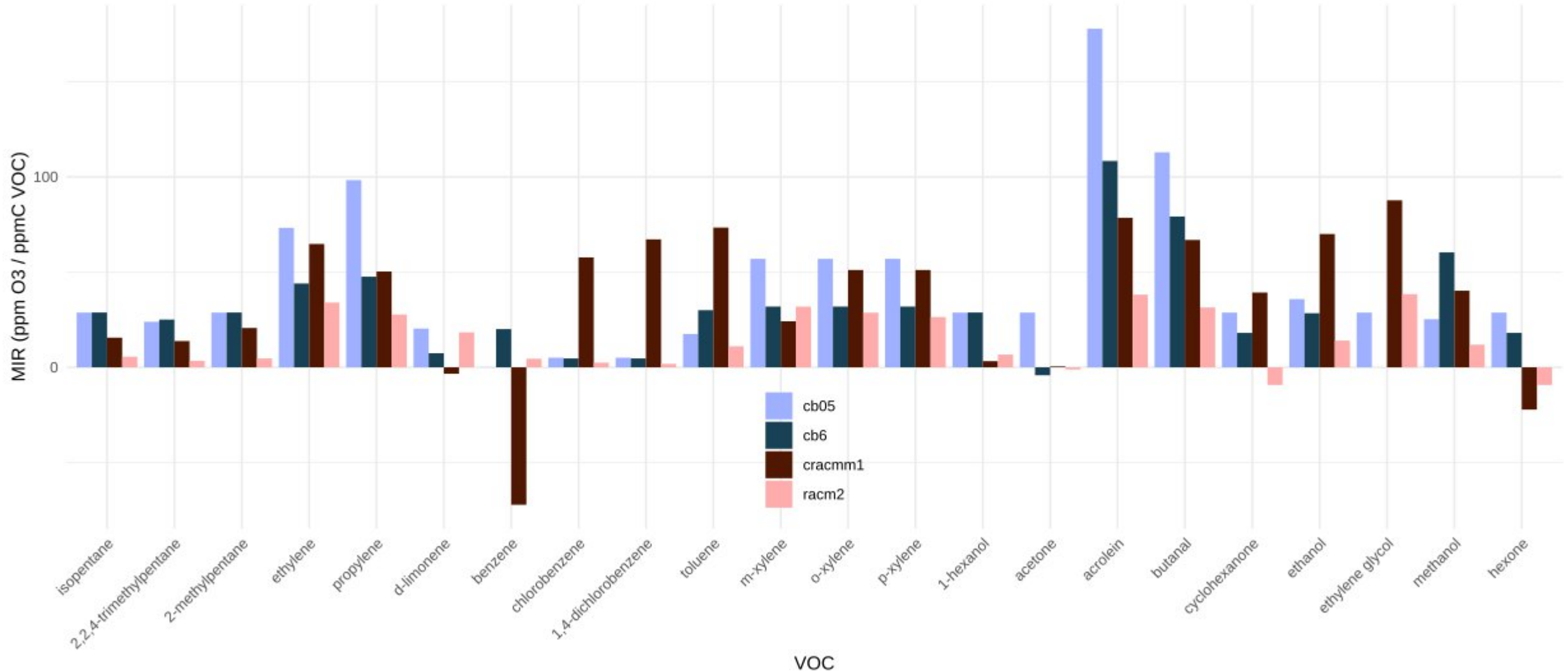
Testing in Barcelona: CB05 vs CB6



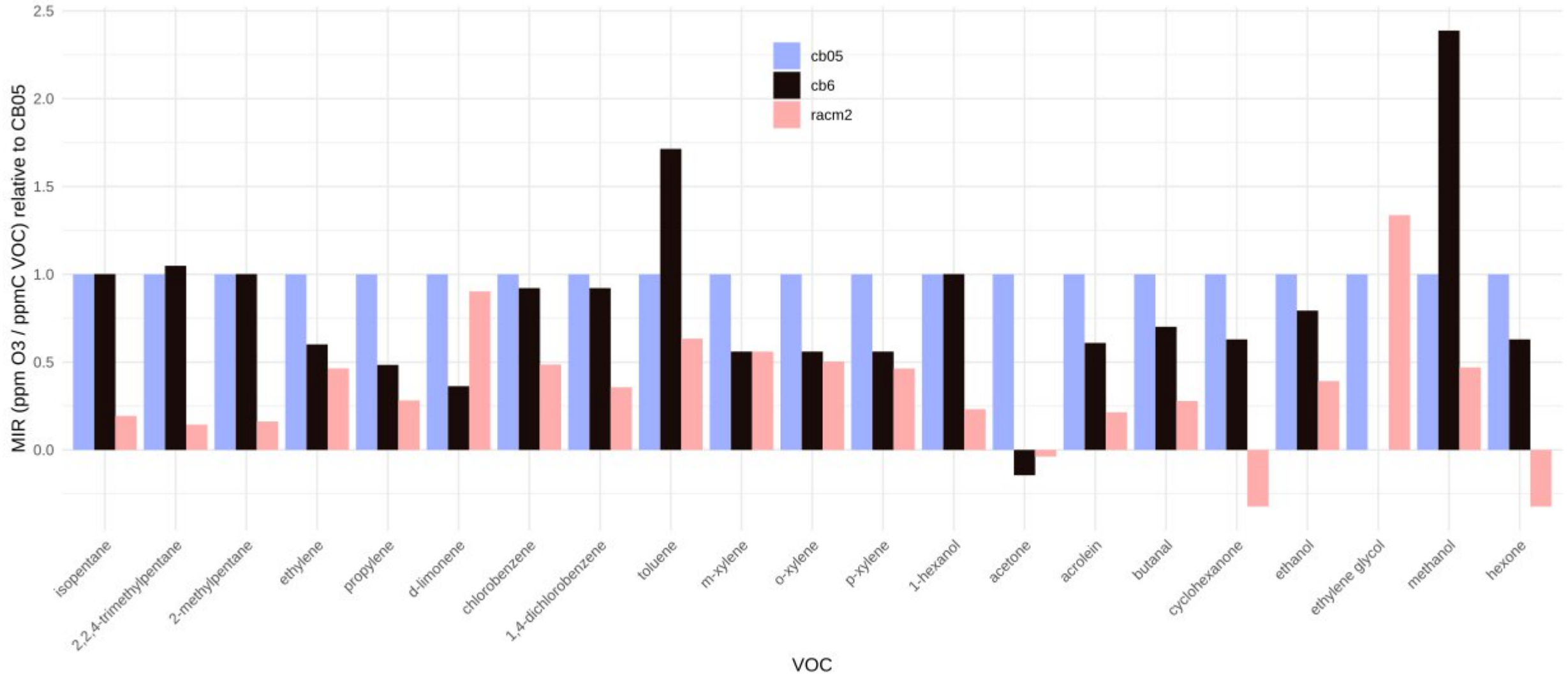
Testing in Barcelona: CB05 vs CB6 vs CRACMM1



Testing in Barcelona: CB05 vs CB6 vs CRACMM1 vs RACM2



Testing in Barcelona: CB05 vs CB6 vs ~~CRACMM1~~ vs RACM2



Summary and Next Steps

- The choice of chemical mechanism is crucial when predicting the impact of VOC emissions changes.
- The Maximum Increased Reactivity scale is a well-known tool that can be used to quantify different mechanisms ozone sensitivity.
- Preliminary results highlight significant differences in mechanisms O₃ responses to VOC emission changes.
- Investigation of differences: need to look into mechanisms as well as HERMES aggregation tables
- Can this be extended to SOA? Sensitivity to both gas mechanism and SOA parametrization



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Thanks for your attention

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