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Modelling activities towards the design of ozone mitigation strategies in Spain

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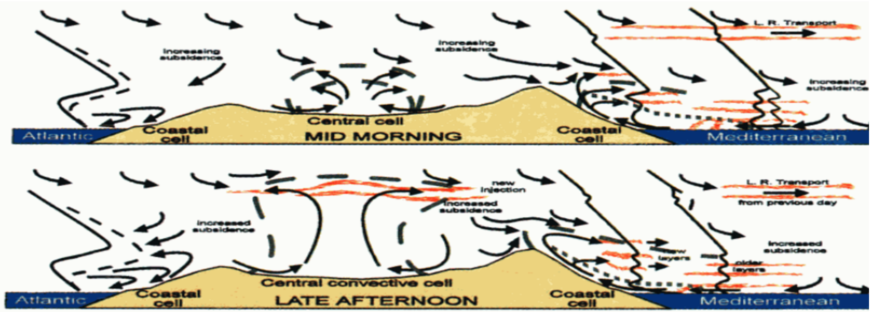
23nd EMEP Task Force on Measurement and Modelling Meeting

Outline

- Background and motivation: O_3 plan for Spain
- Modelling tools
- Source Apportionment of O3 in Spain
- Ozone Plan: emission scenarios and base case run

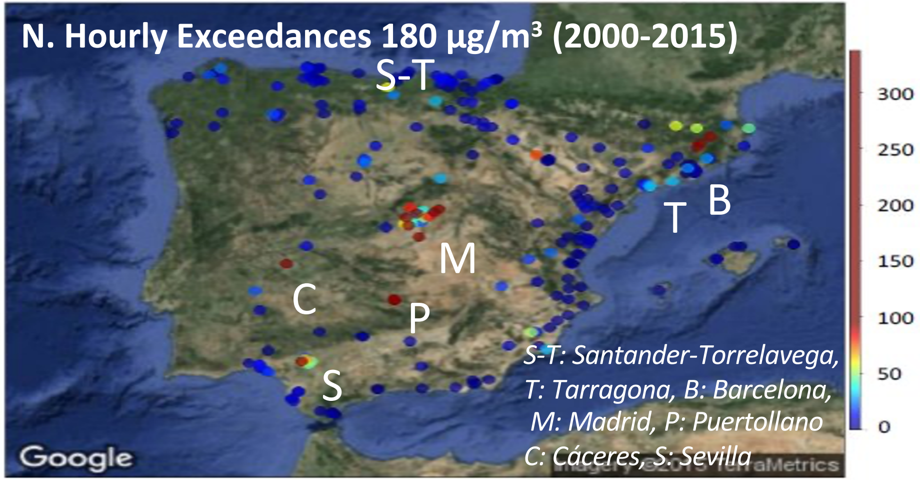
Background and Motivation

O_3 dynamic



Sources: Millán et al., 1997, 2000, 2014; Gangoiti et al, 2001, 2002, 2006; Toll and Baldasano, 2000

O_3 Trends and exceedances



Source: Querol et al. (2016).

Open questions:

- What are the key sources responsible for the high O_3 concentration in Spain?
- Can administrations implement control strategies that are effective to reduce high O_3 concentration?

O_3 plan for Spain

- Advancing our understanding of key processes controlling tropospheric O_3 formation and development of episodes combining monitoring and modelling techniques:
  - Role of emission sectors (source apportionment techniques)
  - NOx/VOCs regimes
  - Better understanding of NMVOCs O_3 formation potential
  - Understanding foreign contributions (source apportionment techniques)

- Designing emission reduction scenarios
  - New emission inventory for 2019 based on MITERD information
  - Emission scenario of MITERD planned mitigation measures
  - Emission scenario of further specific measures: sensitivity runs

- Multi-model air quality modelling at high-resolution

- ***Scientific recommendations for MITERD O_3 plan***

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Modelling tools

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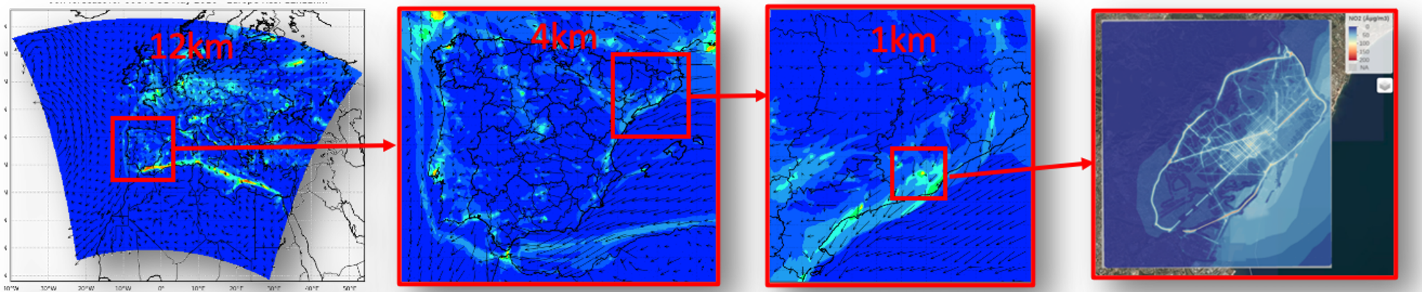
Modelling tools



Pay et al. (2011; 2012 AE) | Baldasano et al. (2012 AE) | Pay et al. (2014 GMD) | Benavides et al. (2019 GMDD)

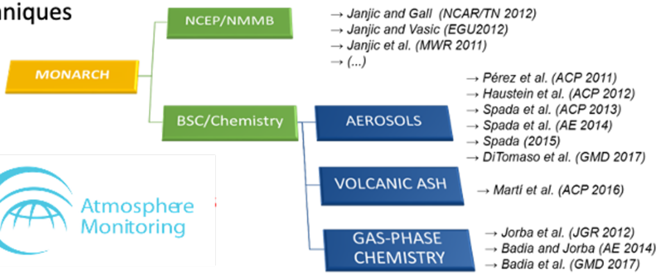
CALIOPE system: air quality forecasts from regional to local scales

In-house model developments

MONARCH model

Multiscale Online Nonhydrostatic Atmosphere Chemistry model

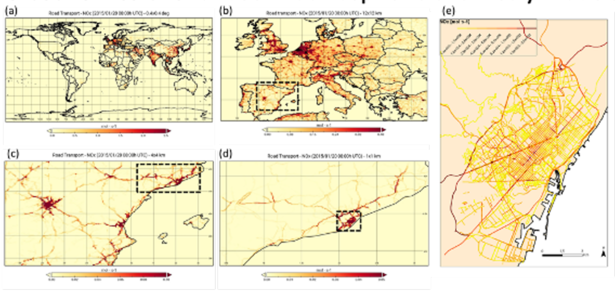
- **Multiscale**: global to regional (up to 1km) scales allowed
- Fully ***on-line*** coupling: weather-chemistry feedback processes allowed
- Enhancement with a ***data assimilation*** system and machine learning techniques



Atmosphere Monitoring

HERMESv3 emission model

A **python-based, open source, parallel and multiscale** emission modelling framework that **processes and estimates gas and aerosol emissions** for use in atmospheric chemistry models.



Guevara et al. (2019, 2020)

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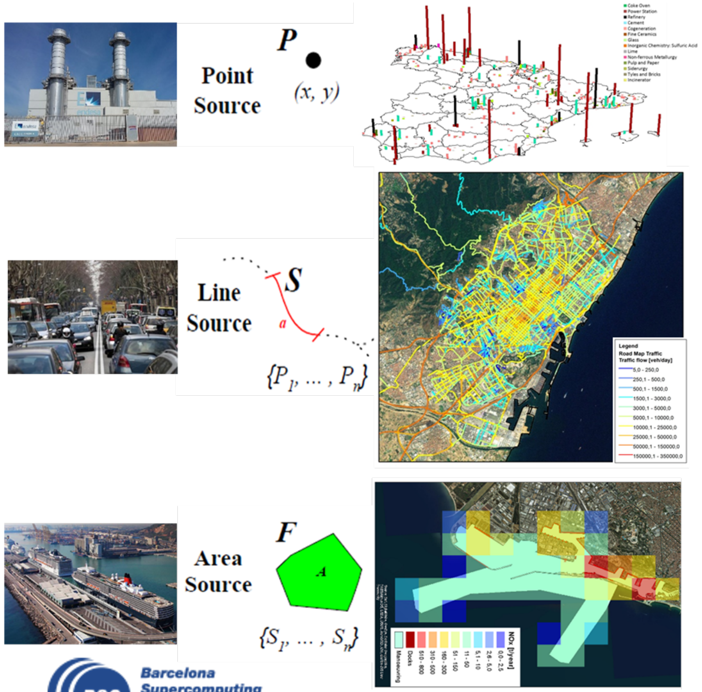
HERMESv3 Bottom Up Model

An **emission model** to estimate emissions at the source level (e.g. road link) combining state-of-the-art **bottom-up methods** with **local activity, emission factors and meteorology**



Multiple sources of information

NO_x, CO, SO_2, NMVOC, NH_3, PM_{10}, $PM_{2.5}$

Guevara et al. (2020)

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Source apportionment of O_3 in Spain: country and sector level

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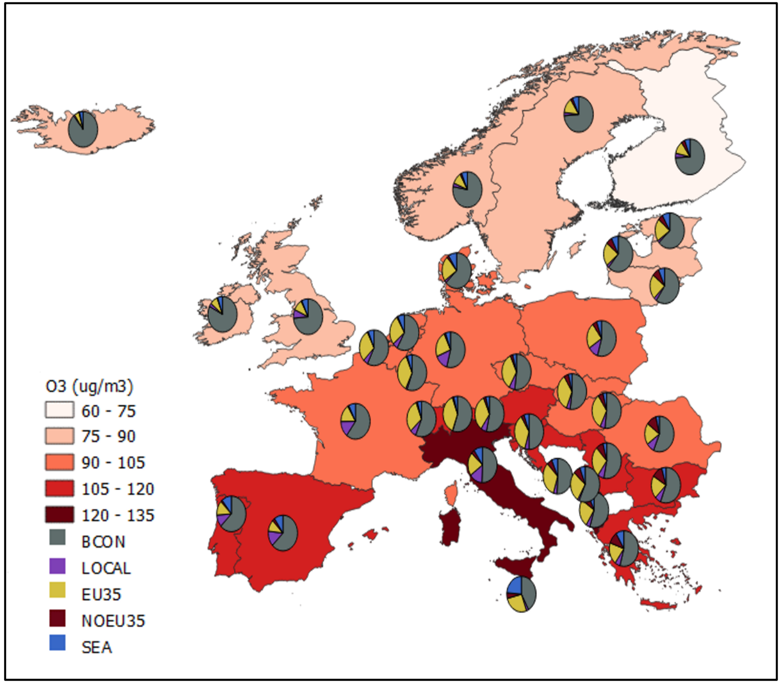
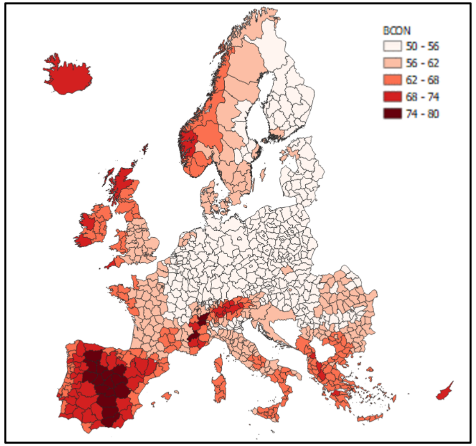
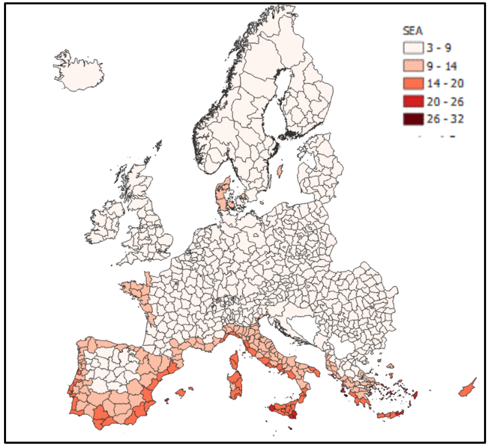
Country vs foreign contributions



Important hemispheric contribution - vertical mixing processes



Relevant role of shipping emissions



2015-2016-2017 MJJAS Mean MDA8 O_3

CMAQ-ISAM SA system

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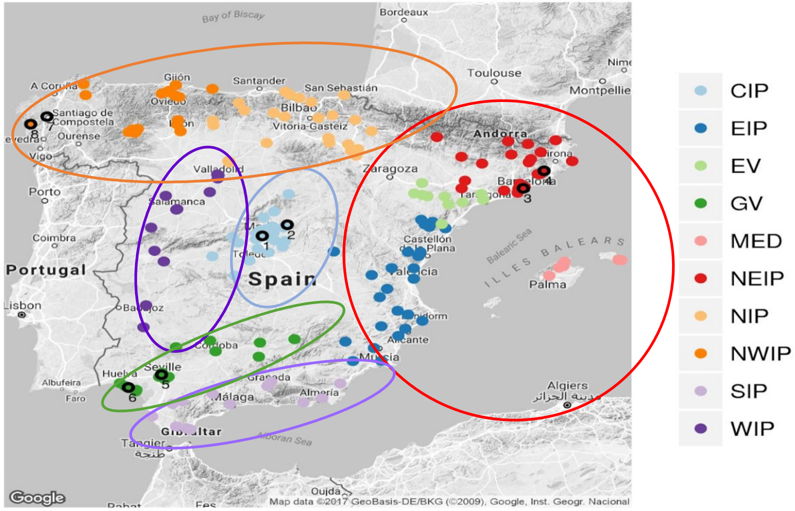
Garatachea et al. (2022 in prep)

Source-sector regional contribution

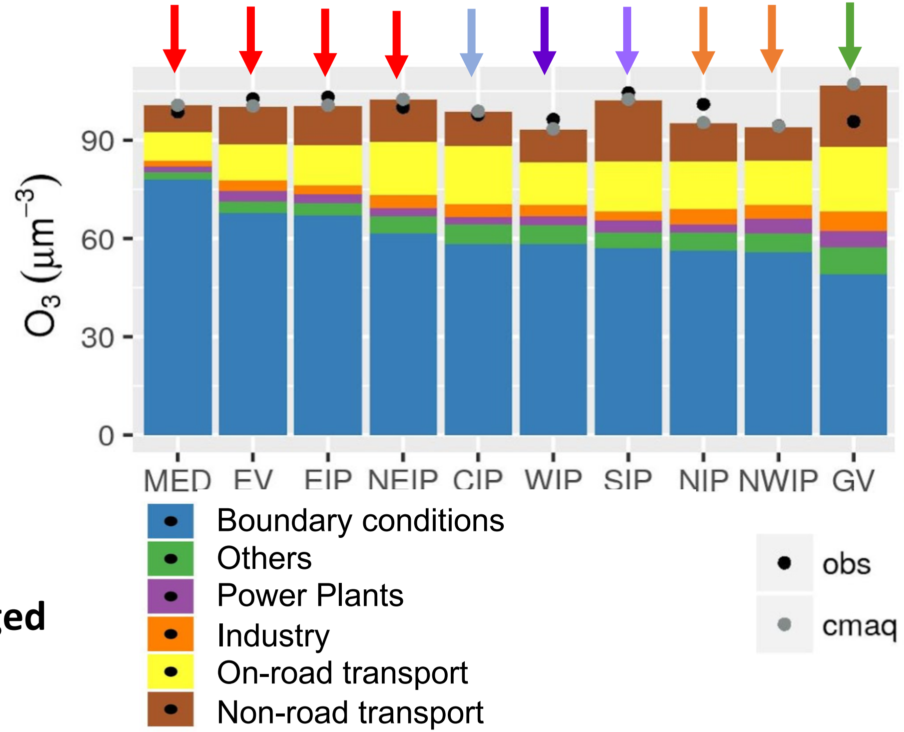
Pay et al. (2019 ACP)



CMAQ-ISAM SA system

NOx/VOCs tagged sources

Daily mean contribution during MDA8 > 120 μ/m³



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O_3 plan for Spain: emission scenarios and baseline modelling results

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Emission scenarios

Scenario	Description	Key sectors	Period model runs
Baseline (EB)	Reference year 2019, combine HERMESv3 (BSC bottom-up emissions for Spain) + MITERD (LPS, PRTR-Spain, fleet composition, official use of solvents)	All	April – September 2019 / 2015 (impact warmer meteorology)
Planned MITERD measures (EP)	EB + measures considered in national MITERD plans (emission reduction consistent with projected data 2030 CLRTAP)	On-road transport, Energy industry, Manufacturing industry, Solvents use, Shipping	April – September 2019 / 2015 (impact warmer meteorology)
Additional specific measures (EE)	**EP + additional emission reduction measures not planned and tailored to reduce O_3 (sensitivity tests)**	On-road transport, Energy industry, Manufacturing industry, Solvents use, Shipping	**July month, focus regional air basins with O_3 issues**

Understand O_3 sensitivity to multiple emission reductions across different regions to identify critical sectors/sources for the design of further emission reductions measures (e.g., field campaigns industry emissions, better constrain emissions)

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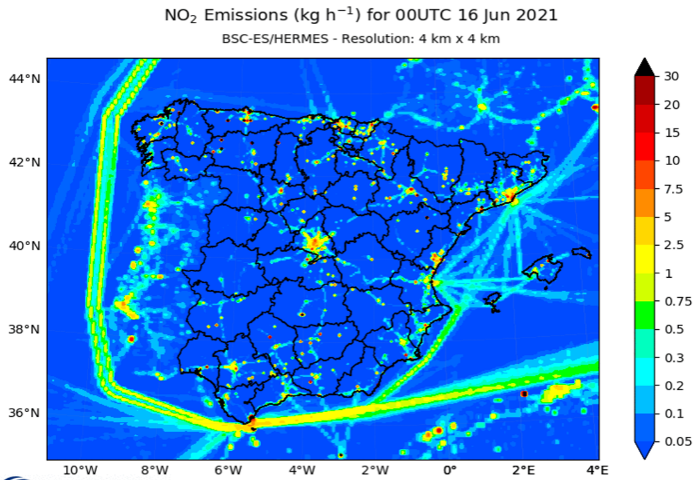
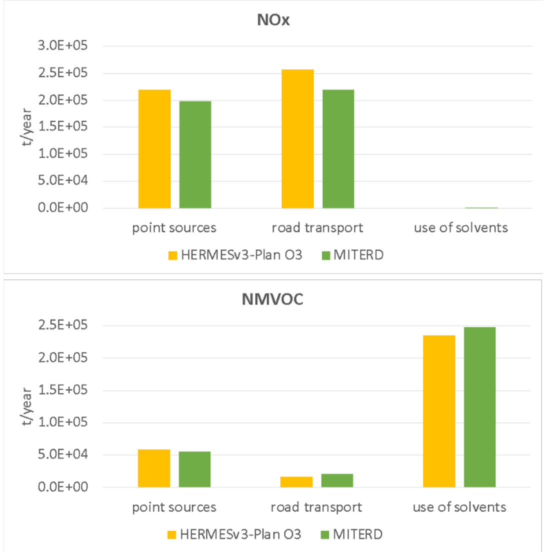
Baseline scenario

- **Spain**: HERMESv3 (Guevara et al., 2020) – bottom-up high resolution emissions
  - Reduction of the inconsistency with official Spanish NOx and NMVOC emissions by integrating the following national datasets into the HERMESv3 system:
    - LPS and PRTR Spain point source emissions
    - Vehicle fleet composition profiles per province
- **Other countries + shipping**: CAMS-REG-AP_v4.2 inventory (Kuenen et al., 2022)





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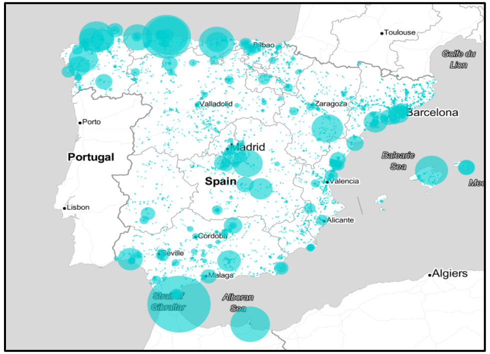
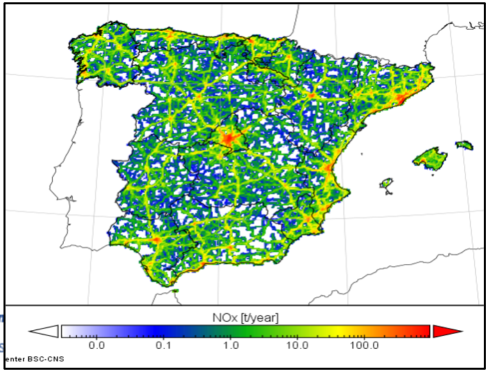
Baseline scenario

Detailed spatial and temporal distribution of emissions

NOx annual industrial emissions

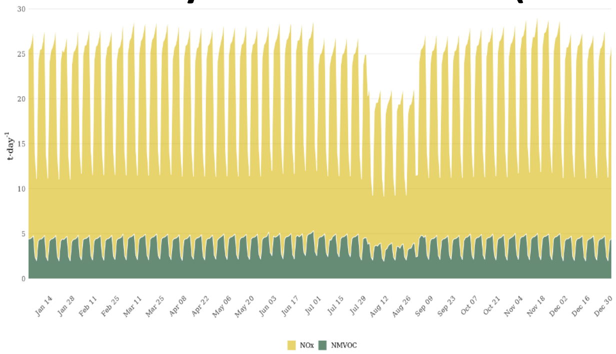


NOx annual traffic emissions



NOx monthly industrial emissions (per branch)

NOx/NMVOC daily traffic emissions (Madrid city)



Scenario with Planned Measures

Implementation in HERMESv3 of emission changes reported by the **official projections data under the CLRTAP** (very complex process due to aggregation level of reporting)

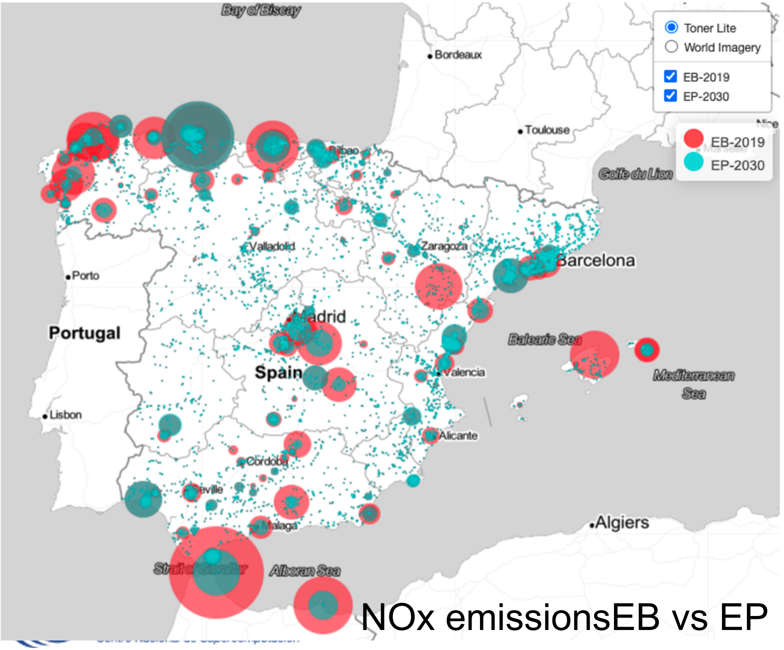
Limitation -> Projected increase of NMVOC from biomass power plants cannot be included as **location of facilities is still unknown (emissions for reporting vs. emissions for modelling**)

		Projected emissions (kt) NOx Guidelines Reporting Years					Projected emissions (kt) NMVOC Guidelines Reporting Years				
NFR Code	**Longname**	**2019**	**2020**	**2025**	**2030**	**DIFF**	**2019**	**2020**	**2025**	**2030**	**DIFF**
1A1	Energy industries (Power plants & Energy Production)	55.6	53.9	47.0	38.9	**-30%**	10.3	10.6	11.2	12.9	**26%**
1A2	Manufacturing Industries and Construction (Combustion including Mobile)	110.8	106.4	84.0	76.8	**-31%**	20.8	20.8	21.0	21.4	**3%**
1A3b	Road Transport	211.2	207.1	175.5	82.7	**-61%**	20.2	21.1	25.0	23.2	**15%**
1A3bi	*R.T., Passenger cars*	126.5	124.0	99.6	16.1	-87%	5.3	5.2	4.8	5.4	3%
1A3bii	*R.T., Light duty vehicles*	22.3	21.9	18.7	16.6	-25%	0.4	0.4	0.3	0.3	-27%
1A3biii	*R.T., Heavy duty vehicles*	60.5	59.1	54.3	47.7	-21%	1.3	1.2	1.2	1.1	-16%
1A3biv	*R.T., Mopeds & Motorcycles*	1.9	2.1	2.8	2.3	18%	11.4	12.3	16.6	13.5	19%
1A3bv	*R.T., Gasoline evaporation*	NA	NA	NA	NA		1.8	2.0	2.0	2.9	60%
1A3d	National navigation (Shipping)	40.8	35.8	24.0	23.2	**-43%**	1.8	1.7	1.3	1.4	**-25%**
2D, 2G	Solvent & other product use	0.1	0.1	0.1	0.1		257.6	256.9	248.8	244.5	**-5%**

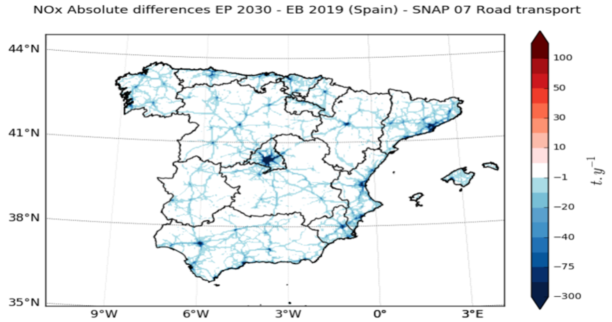
Scenario with Planned Measures

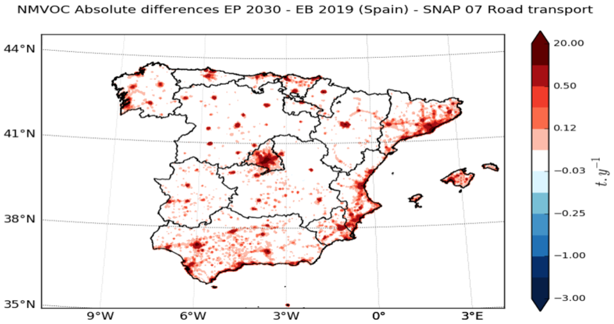
Heterogeneous impact across sources:

- Shut down of coal fired power plants vs. increase of emissions natural gas power plants
- Urban areas: heavy reduction of NOx and slight increase of NMVOC



NOx emissionsEB vs EP

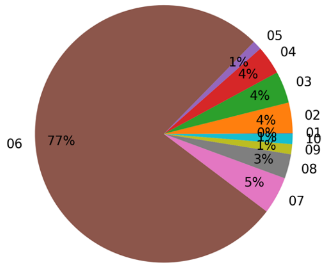




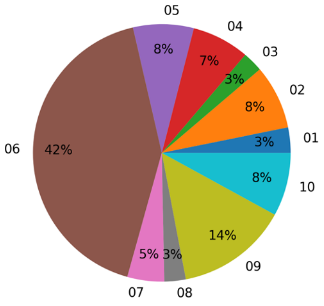
Specific measures: NMVOCs emissions ozone formation potential

NMVOC emissions:

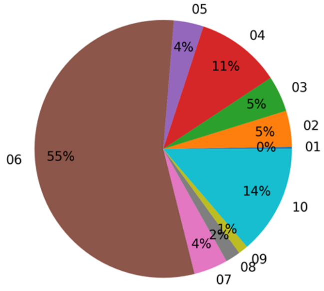
Madrid



Andalucia



Catalunya



SNAP sectors:
01 Combustion in the production and transformation of energy
02 Non-industrial combustion plants
03 Industrial combustion plants
04 Industrial processes without combustion
05 Extraction and distribution of fossil fuels
06 Use of solvents and other products
07 Road Transport
08 Other mobile sources and machinery
09 Waste treatment
10 Agriculture

- To obtain the NMVOC speciated inventory and to calculate the Ozone Formation Potential (OFP):

$$E_i = \sum_j E_j \times R_{ij}$$

where, i is a specific NMVOCs species, j is the emission source, is the total emission of the species i, is the total emission of the source j, and is the ratio of species i to source j

$$OFP_i = \sum_j E_{ij} \times MIR_i$$

where OFP_i is the total ozone formation potential of species i, E_{ij} is the emission of the species i for source j, and MIR_i is the maximum increment reactivity of species i (g O_3 / g VOC).

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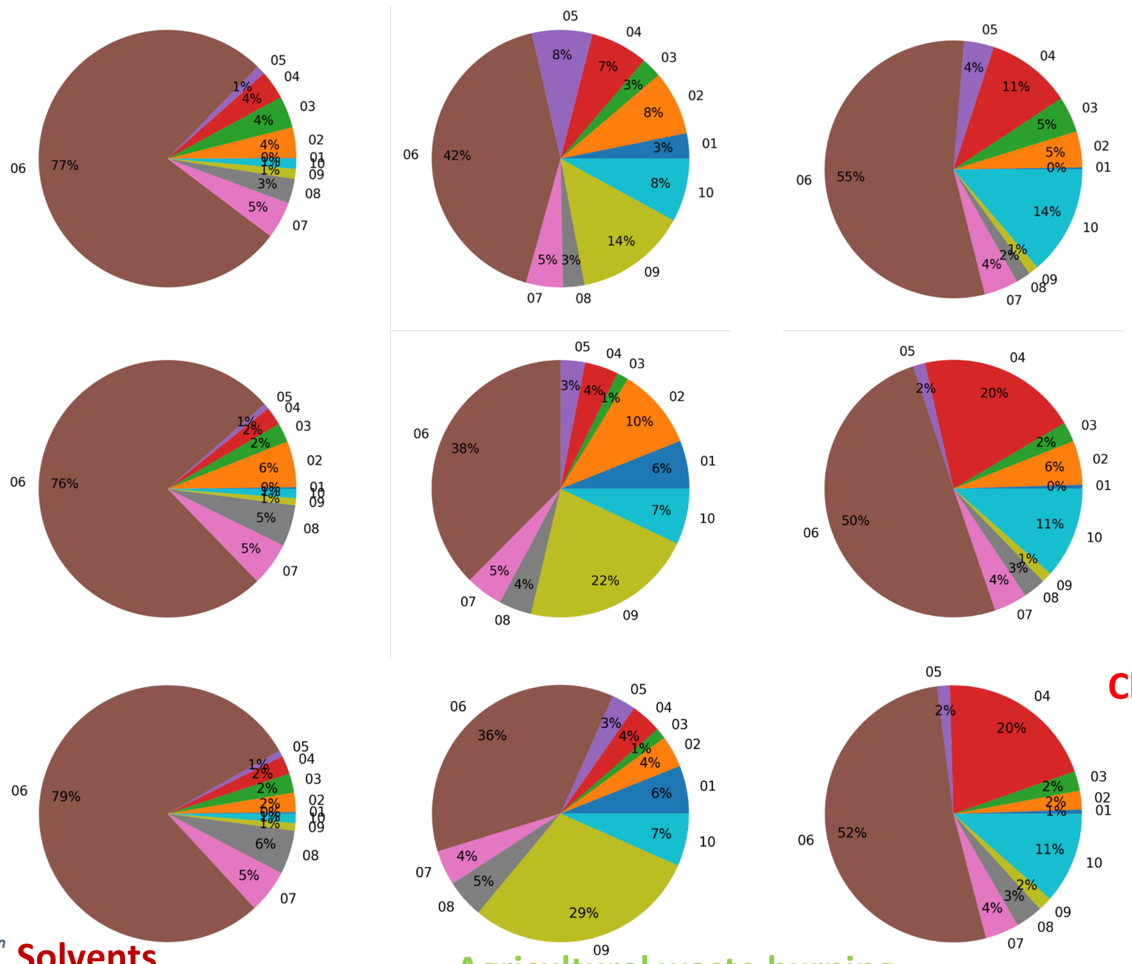
NMVOC emissions:

OFP annual:

OFP June-August



Solvents

Agricultural waste burning

Chemical industry

SNAP sectors:

01 Combustion in the production and transformation of energy
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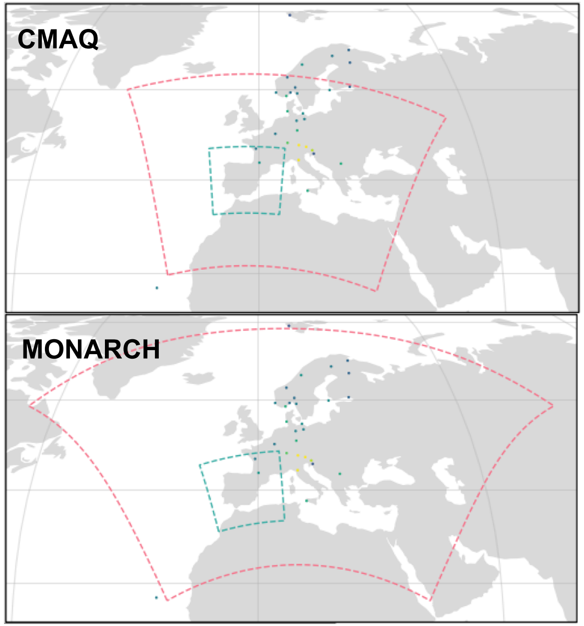
Air quality Models and setup

- 2 models (robustness in sensitivities and model uncertainty): **WRF-CMAQ, MONARCH**
- Same anthropogenic emissions: CAMS-REG-ANT-v4.2 (Europe), HERMESv3 bottom-up (Spain)
- Period of study April-September 2019 (focus June-July-August)

Model	**CMAQ**	**MONARCH**
Domains	Europe (12km)/Spain (4km) Lambert Conformal Conic	Europe (20km)/Spain (5km) Rotated latitude-longitude
	37 vertical layers (top 50 hPa)	24 vertical layers (top 50 hPa)
Meteorology (BC)	WRFv3.5 (FNL)	NMMB (ERA5)
Chemistry (BC)	CMAQv5.0.2 CB05 + AERO6 (CAMS)	Online CB05 + BSC aerosols (CAMS)
Natural emissions	MEGAN (biogenic)	MEGAN (biogenic) + GFAS



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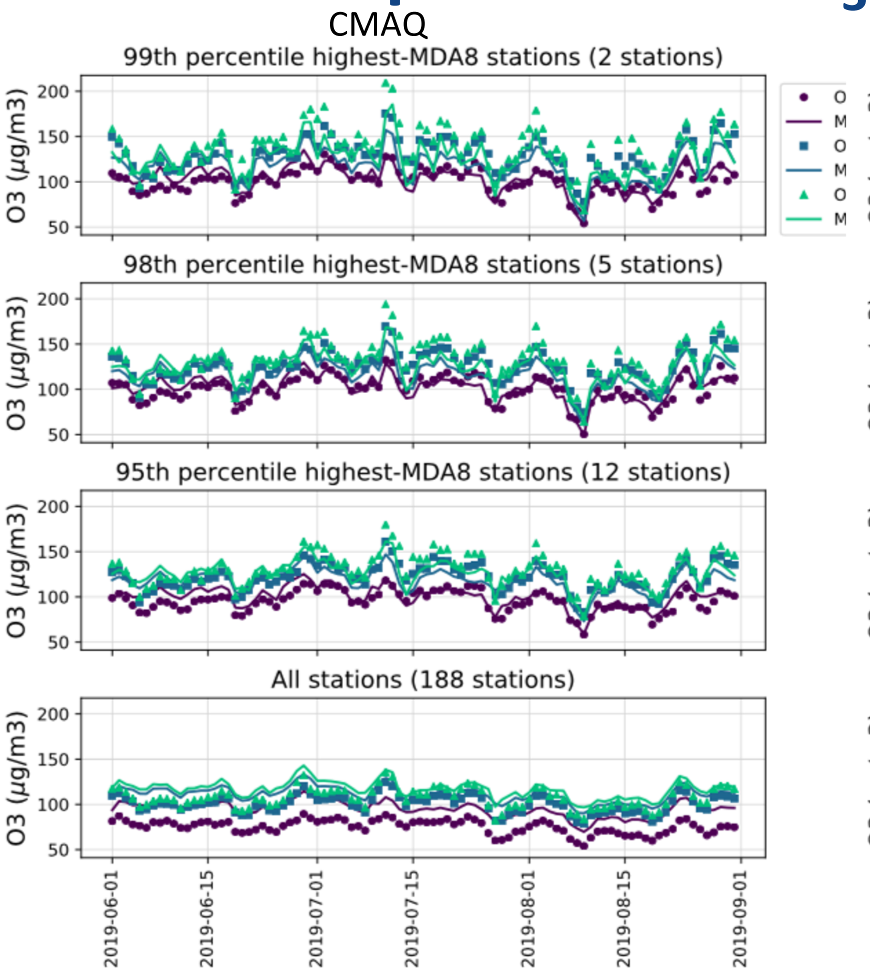
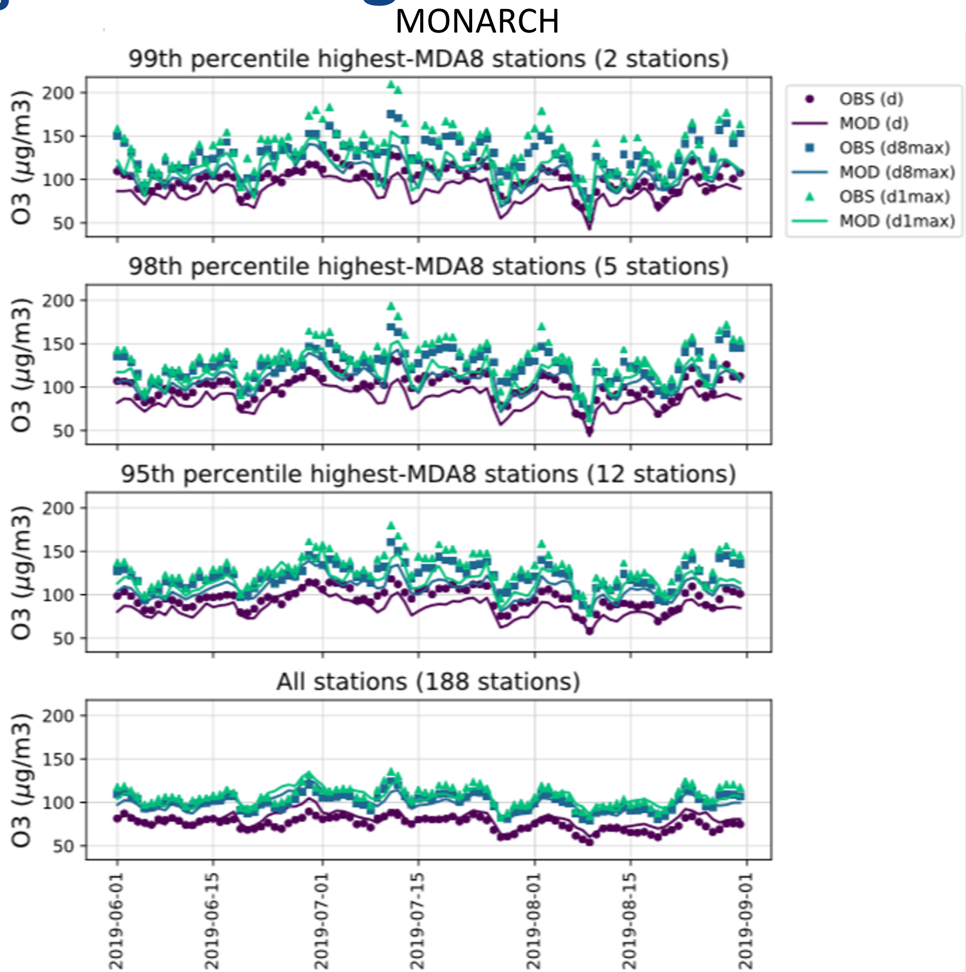
General statistics – comparison reference CTMs

CMAQ	MB	nMB	RMSE	nRMSE	PCC	slope	nMSDB	N	Mo	Mm
h	18.97	25.99	28.80	39.47	0.69	0.51	-26.56	586669	72.98	91.94
d	18.94	25.96	24.15	33.09	0.66	0.54	-18.88	24478	72.98	91.92
d1max	9.67	9.32	20.84	20.10	0.69	0.53	-23.70	24478	103.69	113.36
d8max	11.28	11.65	20.20	20.86	0.68	0.50	-25.40	24149	96.86	108.14
MONARCH	MB	nMB	RMSE	nRMSE	PCC	slope	nMSDB	N	Mo	Mm
h	5.03	6.89	24.43	33.47	0.62	0.48	-23.03	586669	72.98	78.00
d	4.97	6.81	16.36	22.42	0.63	0.49	-21.24	24478	72.98	77.95
d1max	-0.58	-0.56	19.18	18.50	0.67	0.53	-20.90	24478	103.69	103.11
d8max	-0.05	-0.05	16.53	17.07	0.69	0.52	-24.75	24149	96.86	96.81
EMEP	MB	nMB	RMSE	nRMSE	PCC	slope	nMSDB	N	Mo	Mm
h	5.64	7.77	22.78	31.38	0.68	0.41	-39.51	541924	72.61	78.25
d	5.65	7.79	16.86	23.22	0.59	0.35	-40.20	22605	72.59	78.25
d1max	-6.85	-6.64	20.98	20.33	0.63	0.37	-41.86	22605	103.23	96.38
d8max	-3.03	-3.15	17.83	18.55	0.64	0.38	-40.53	20987	96.15	93.12
CHIMERE	MB	nMB	RMSE	nRMSE	PCC	slope	nMSDB	N	Mo	Mm
h	16.65	22.85	26.73	36.68	0.72	0.55	-23.96	580417	72.89	89.54
d	16.64	22.84	22.71	31.15	0.61	0.41	-32.96	24217	72.89	89.53
d1max	8.58	8.28	20.65	19.94	0.67	0.43	-36.10	24217	103.61	112.18
d8max	12.41	12.83	20.89	21.60	0.66	0.43	-35.22	23637	96.71	109.11

Temporal series O_3 monitoring stations





Summary

- Ongoing work towards the design of specific measures to reduce the O_3 problem in Spain
- Spain O_3 has significant local contribution compared with other EU states
- Characteristic contribution from vertical mixing (deep convective PBL during summer)
- Updated 2019 emission inventory for modelling applications and designing emission mitigation scenarios - focus on NMVOCs OFP
- Two models with complementary behaviour and sensitivities (positive for robustness)
  - CMAQ: systematic positive bias with better representation of ozone peaks
  - MONARCH: better daily cycle with underestimation of maximum peak values
  - Local/regional air basins well captured by two models
- Next steps: modelling emission scenarios

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Thank you!

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