Thursday 4th

Instrumentation and advances in air quality monitoring

Application of the Decoupled Direct Method (DDM) to support an advanced air pollution assessment system in Madrid (Spain)

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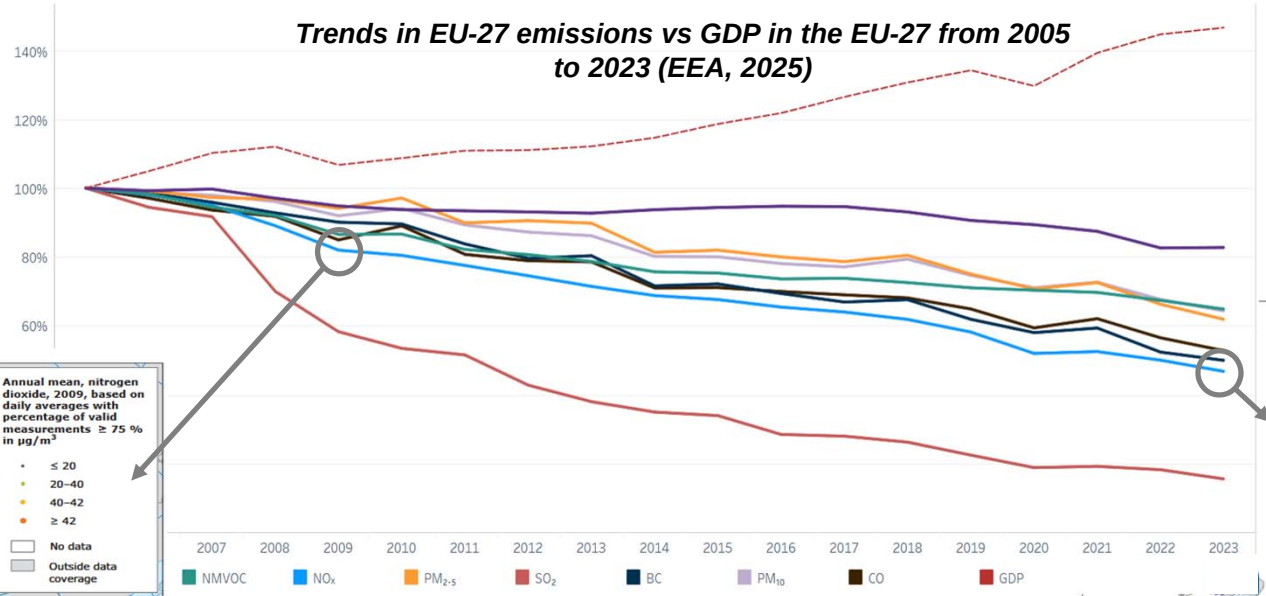
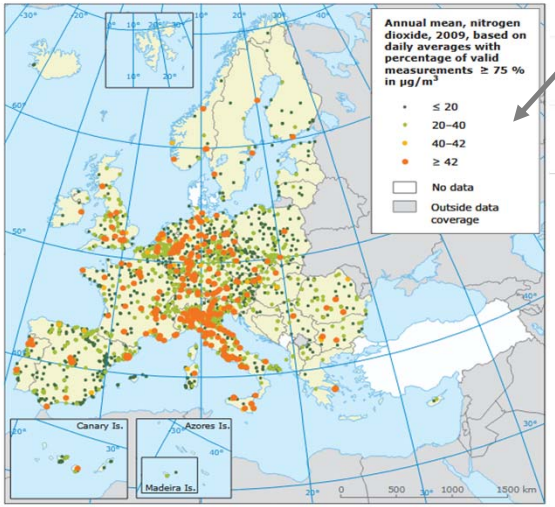
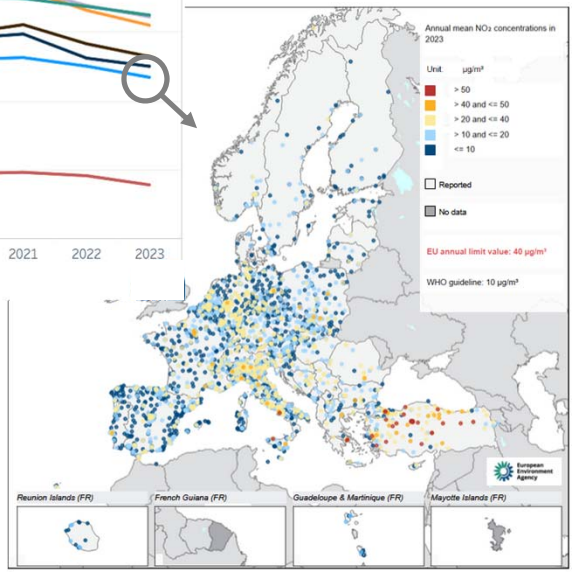
1. INTRODUCTION

- Emissions in Europe are declining and air quality is improving



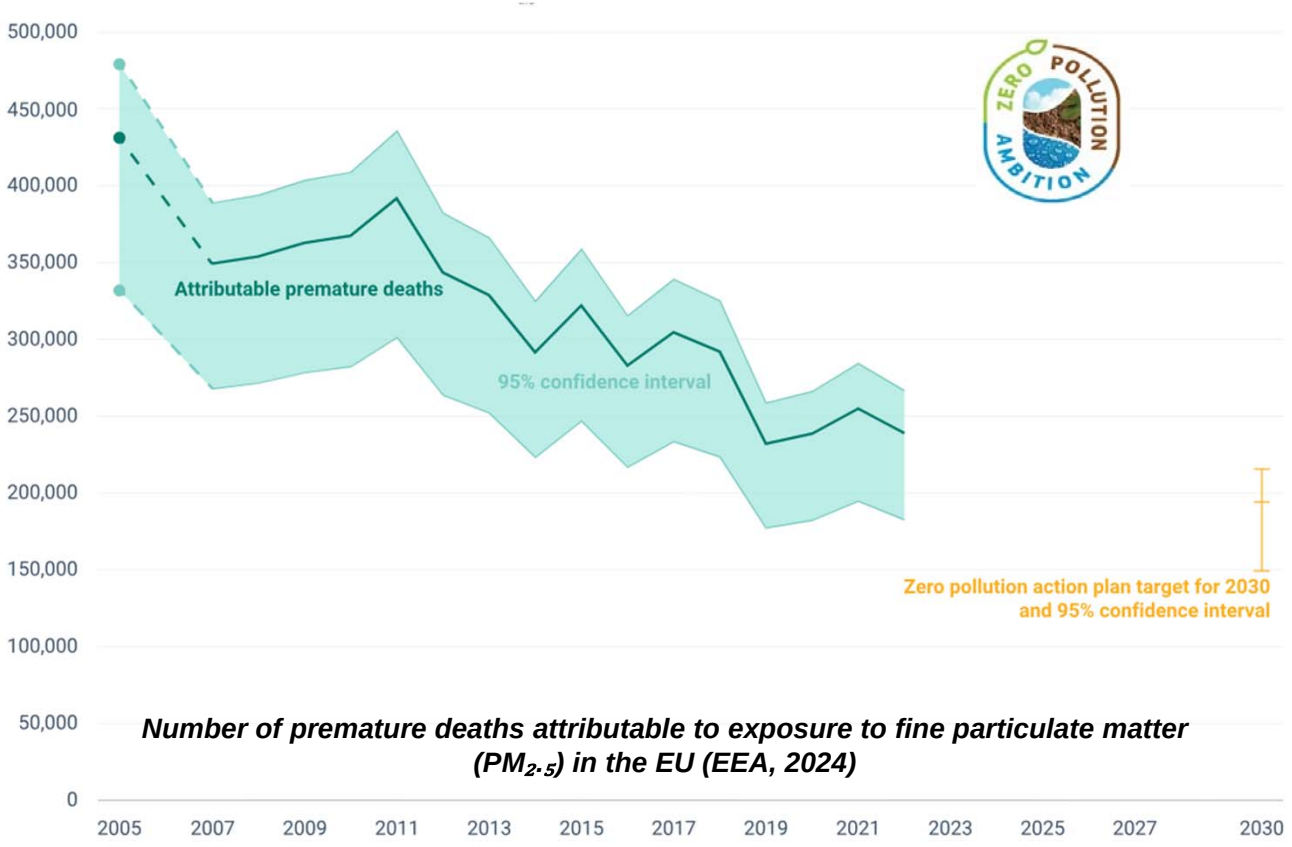


2009 NO_2 annual mean (EEA, 2011)



2023 NO_2 annual mean (EEA, 2025)

- However, air pollution continues to be a major public health issue: over 300,000 attributable premature deaths
- Further action needed to meet interim targets (Directive (EU) 2024/2881) towards a toxic-free environment vision of the European Commission for 2050



Number of premature deaths attributable to exposure to fine particulate matter ($PM_{2.5}$) in the EU (EEA, 2024)

better information systems needed to design further emission reductions and assess progress (emissions, air quality, exposure)

- Advanced air pollution and climate change analysis and assessment system for the city of Madrid (SIMAD)

MADRID → Informed decision making

Exposure assessment

NOMMON → Pedestrian fluxes

Anonymized mobile network massive data

Origin-destination (OD) matrices

aimsun.

Dynamic (CDRs-based) approach

Total daily exposure (µg·m⁻³·person ·h)

POLITÉCNICA

tarindustrial

Concentration

Link-level traffic data → Emission computation → Reduced form model

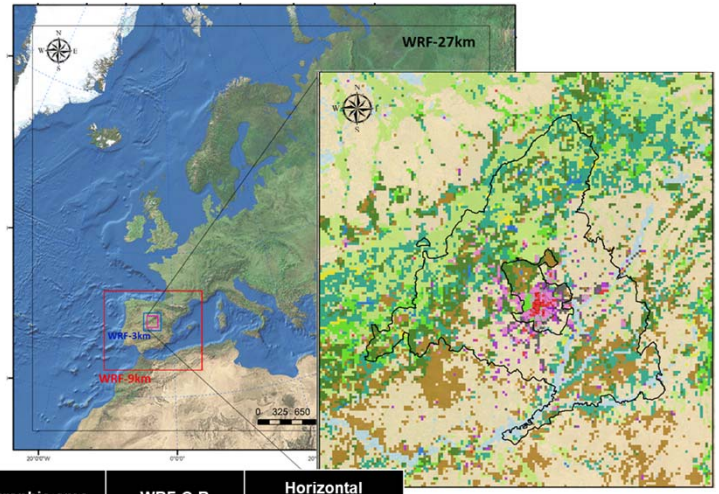
$$C_{i,h} = C_{i,0,h} + \Delta BC \cdot S_{BC,i} + \sum_{j=1}^{J}\sum_{k=1}^{K} \Delta e_{j,k} \cdot S_{i,j,k,h}$$

Source apportionment

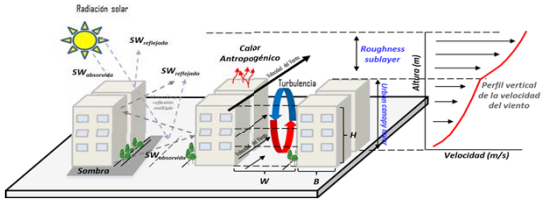
CMAQ-DDM 3D

2. METHODOLOGY

- CMAQ 5.4 annual simulation (base year = 2022)



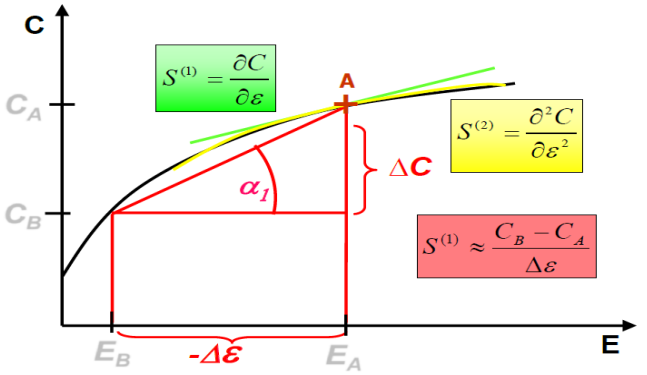
Domain	Geographic area	WRF C-R	Horizontal resolution (km)
D1	Europe	248 x 220	27 x 27
D2	Iberian Peninsula	159 x 129	9 x 9
D3	Spain central area	84 x 87	3 x 3
D4	Greater Madrid area	159 x 168	1x1



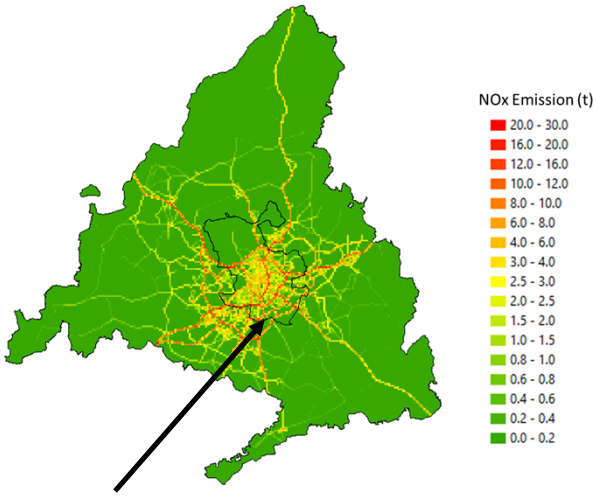
- Meteorology from WRF-BEP (4.2.1)
- SMOKE emission processing (4.8.1)

Option	D4 set-up
Secondary Inorganic aerosol	ISORROPIA II (Fountoukis, C and A. Nenes, 2007)
SOA model	SOA (Pye,H. et al., 2017; Murphy,B. et al., 2017)
Aerosol model	AERO6 (3 modes) (Appel et al., 2013)
Aerosol physics	Coagulation/condensation/nucleation
Wet deposition of particles	Jesse Bash, Sarwar et al. (2015)
Gas phase chemistry	CB6 (Emery, 2015)
Landuse database	Same as WRF
Vertical layers	39 fixed terrain following Layers
Vertical extent	17600m
Depth first layer	7.7 m
Forest fires	None
Lightning	Yes (Daiwen Kang)
Sea salt	Gantt, B. et al (2015)
Windblown dust	no
Advection scheme	Horizontal Advection Yamo (Yamartino,1993)
	Vertical Advection WRF
Vertical diffusion	Vertical Diffusion ACM2 (Pleim, 2007)
	Horizontal Diffusion Multiscale
Dry deposition	Model based on Pleim and Ran (2011)
Stomatal resistance	Wesely (1989)
Cloud chemistry	acm_ae6 (Fahey, K.M., 2017)
Coarse nitrate	yes

- Decoupled Direct Method in Three Dimensions (CMAQ-DDM-3D) (Cohan & Napelenok, 2011)
- semi-normalized sensitivity coefficients computed in run time for a given parameter (e.g. any emission subset by sector, precursor and/or geographical area)
- Sectors explicitly considered:
  - Traffic: passenger cars (PC)
  - Traffic: light-duty vehicles (LDV)
  - Traffic: heavy-duty vehicles and buses (HDV)
  - Traffic: taxis (TX)
  - Residential, commercial (RC)
  - Residential, institutional (RI)
  - Use of solvents and other products (SU)



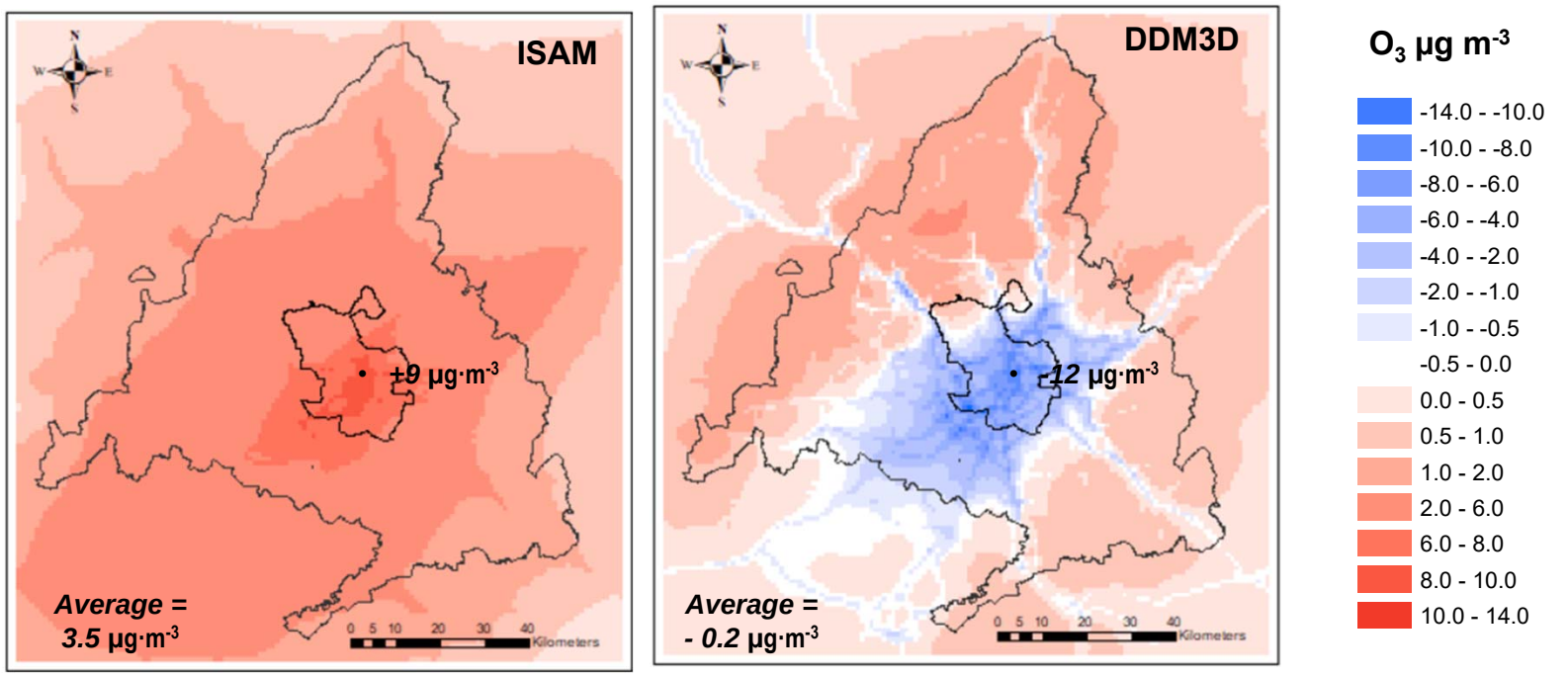
Pollutant (i)	Precursors (j)
NO_2	NO_X
O_3	NO_X, VOCs
$PM_{2.5}$	NO_X, VOCs, SO_2, NH_3, primary $PM_{2.5}$



- Total emissions within the city of Madrid (local emissions)

- Sensitivity coefficients may be considered a **source apportionment** method

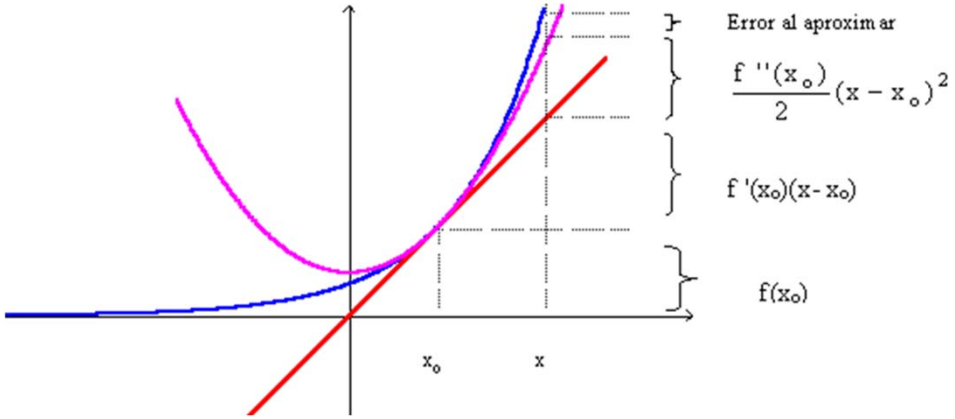
Average contribution of road traffic emissions to O_3 levels in the Madrid region during a summer period



Borge et al., 2024

- Tagging methods (e.g. CMAQ-ISAM) have been proven useful to diagnose un understand complex, non-linear contribution processes
- DDM sensitivities are more informative on emission reduction impacts and thus, anticipate the outcome of potential measures

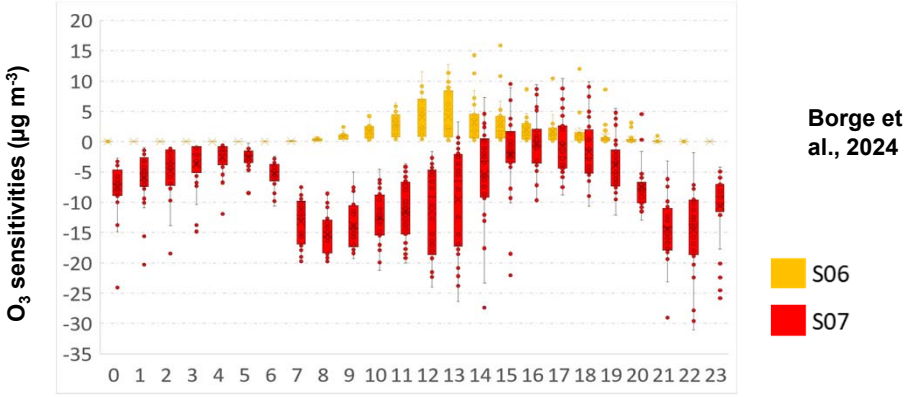
- **Reduced form model** from first-order sensitivities (grid-specific)
  - for each 3-month period (15 representative days)
  - hour-specific average sensitivity



$$f(x) \approx f(x_0) + f'(x_0)\cdot(x-x_0) + \frac{f''(x_0)}{2!}\cdot(x-x_0)^2 + \cdots + \frac{f^{(n)}(x_0)}{n!}\cdot(x-x_0)^n$$

$$f(x) \approx \sum_{i=0}^{n} \frac{f^{(n)}(x_0)}{n!}\cdot(x-x_0)^n$$

- Taylor series expansion neglecting second and higher-order derivatives = DDM sensitivities:



Borge et al., 2024

1-hour concentration of pollutant (i)

corresponding concentration in the baseline simulation

$(J \cdot K = 63)$

$$C_{i,h} = C_{i,0,h} + \Delta BC \cdot S_{BC,i} + \sum_{\substack{j=1 \\ k=1}}^{\substack{J \\ K}} \Delta e_{j,k} \cdot S_{i,j,k,h}$$

Change of boundary conditions (for pollutant i) (0 for short-term scenarios)

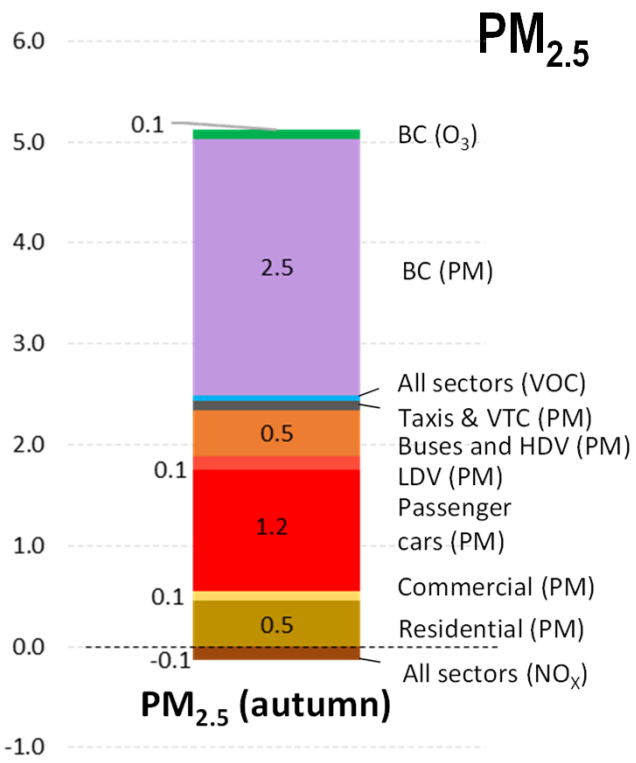
BC sensitivity

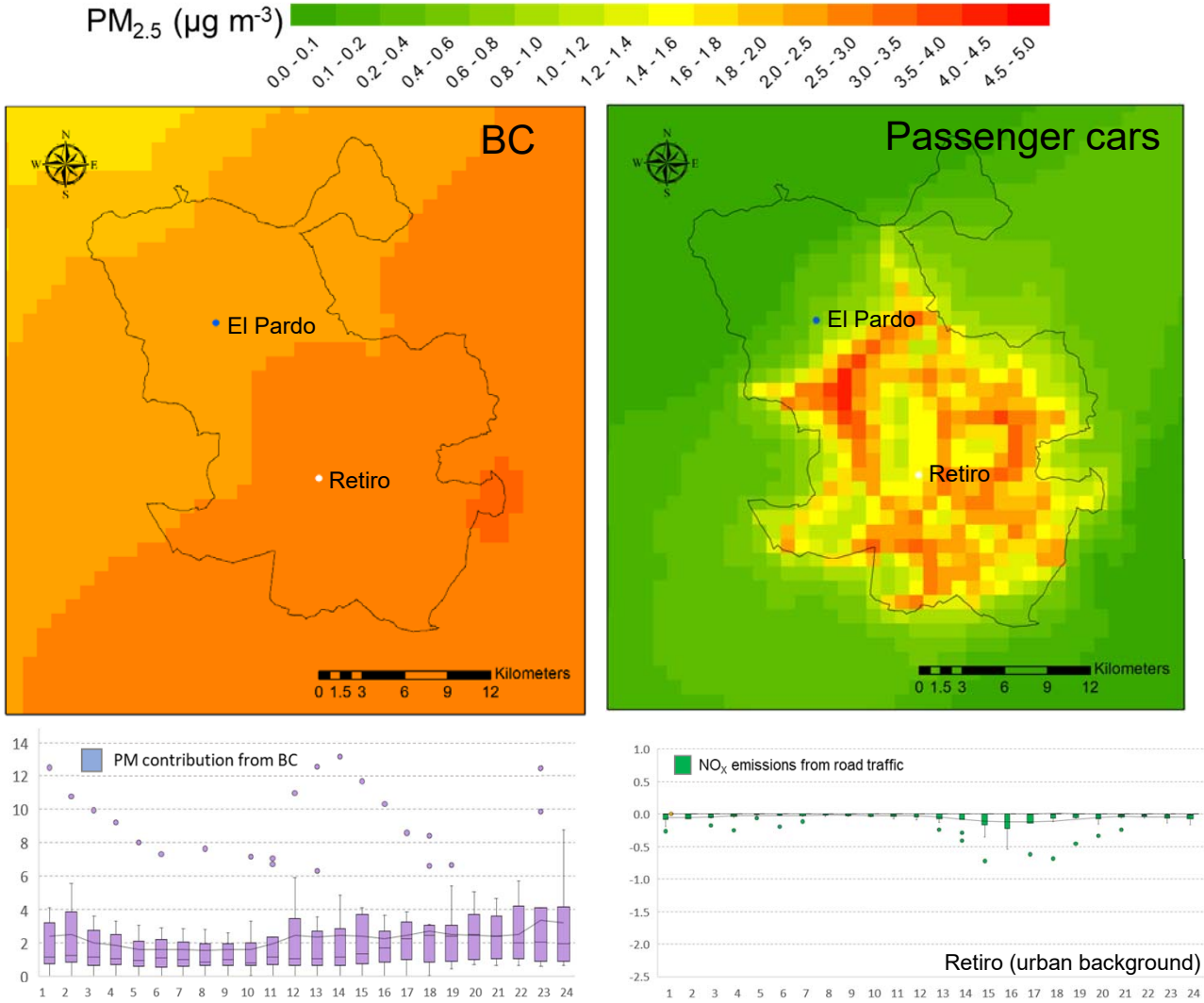
Sensitivity of pollutant (i) concentration to precursor (j) from sector (k) – average for hour (h)-

Emission change of precursor (j) from sector (k)
Prescribed by the user in the scenario module or computed by the emission module

3. RESULTS

3.1. Source apportionment

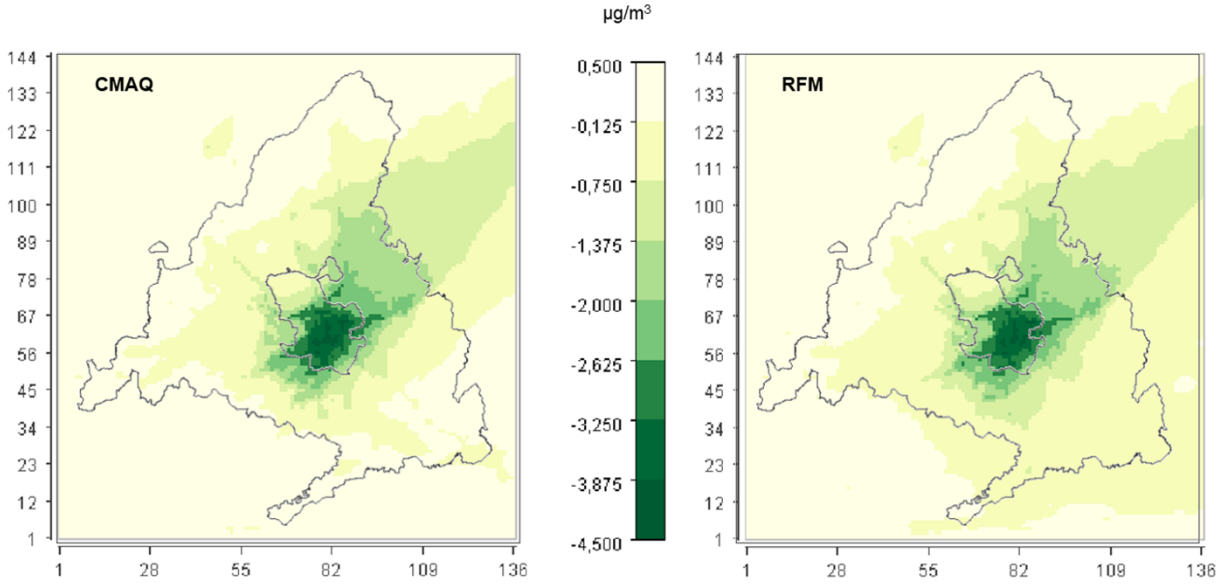




3.2. Reduced form model

• Ability to reproduce CMAQ results for a moderate emission reduction scenario:

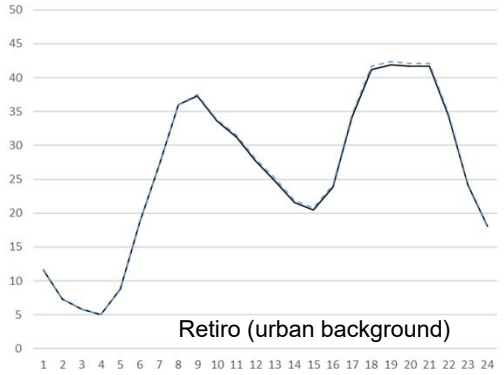
Sector (k)	Δe (all j)
PC	-15%
LDV	-15%
HDV	-15%
RCI	-20%
SU	-5%



Comparison of the response (NO_2) of CMAQ vs RFM for an emission reduction scenario (Borge et al., 2023)

- Very precise results for averaged reductions (within ±1 µg/m³ in all grid cells)
- Temporal variations perfectly captured (r^2 coefficients above 0.99 consistently for all three pollutants)

Hourly average NO_2 concentrations (µg/m³)



MNB = -1.7%

r^2 = 0.997

4. CONCLUSIONS AND FURTHER WORK

- DDM may consistently support source apportionment studies and screening scenario modelling tools at city level
- The reduced model built from DDM first-order sensitivities successfully reproduced the responses of the full CTM under a moderate emission reduction scenario
- Very high informative power for the design of potential measures: specific sensitivities by grid cell, season and hour and precursor

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- Further analysis needed to assess:
  - the sustainability of the SIMAD tool in time
  - capability to support a wide range of simulations to define air quality roadmaps under the Directive (EU) 2024/2881

Instrumentation and advances in air quality monitoring

This study was developed under contract with the Madrid City Council "Advanced air pollution and climate change analysis and assessment system for the city of Madrid " (Nº Expediente: 300/2021/00714 Lote 2, proyecto SIMAD: Simulador Madrid. Clima y Aire)

Thank you for your attention!

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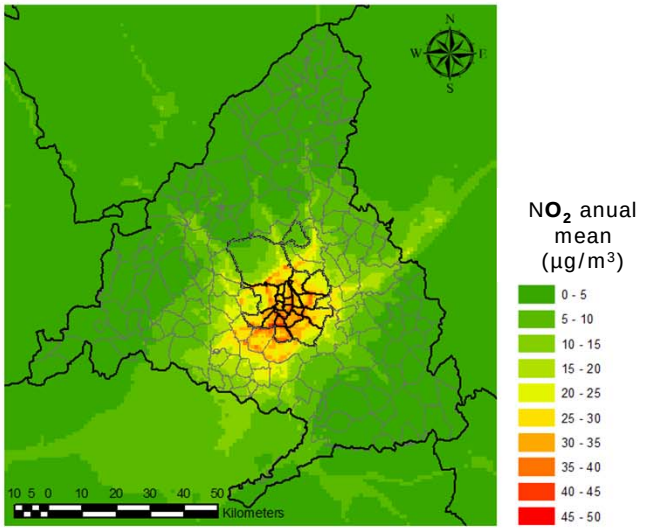
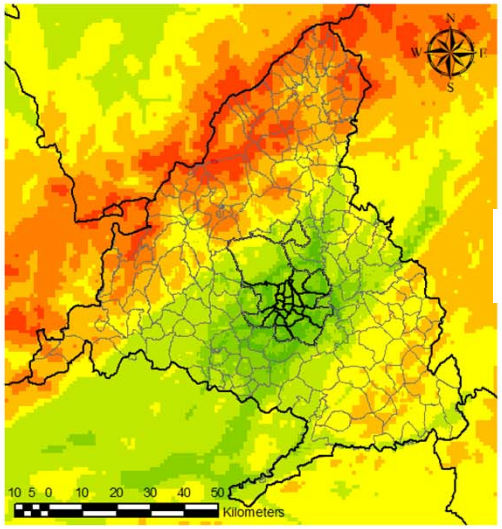
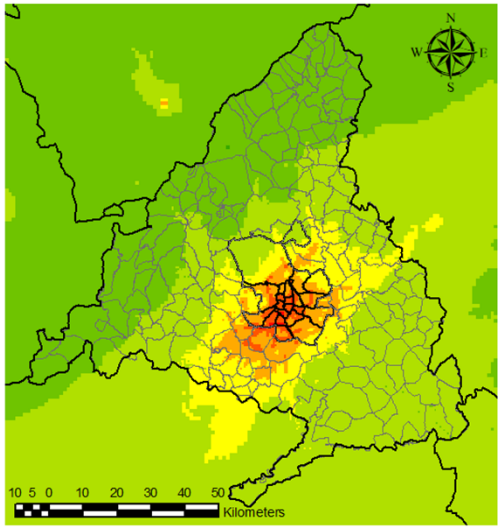
- Acceptable model performance



NO_2 anual mean ($\mu g/m^3$)

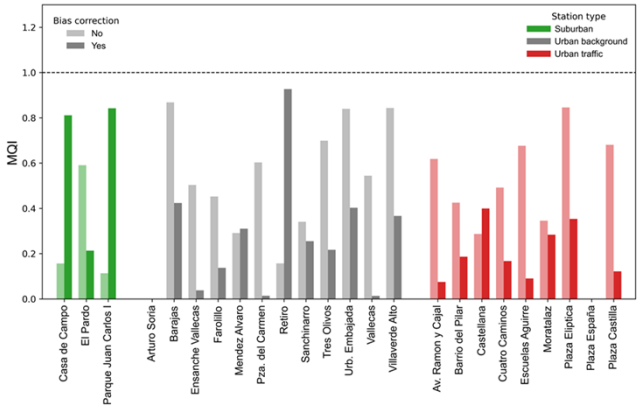


O_3 anual mean ($\mu g/m^3$)

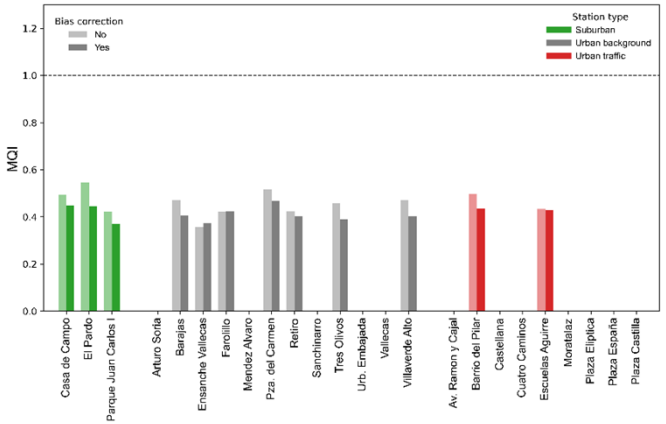
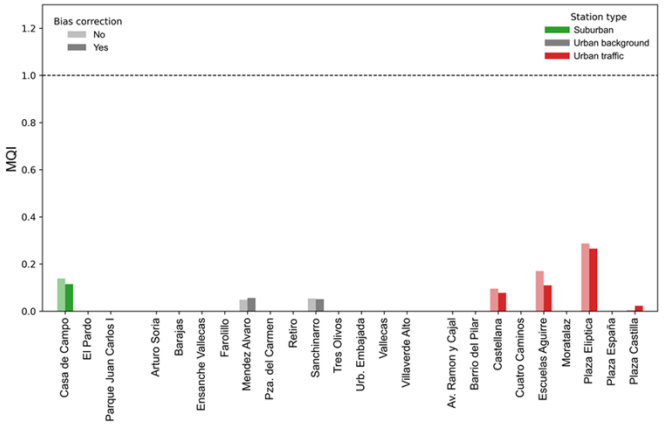


$PM_{2,5}$ anual mean ($\mu g/m^3$)

MQI of annual predictions of NO2



MQI of 8-hour predictions of O3



MQI of annual predictions of PM25