



HERMES_Δ: bridging the gap between official inventories and model-ready emissions for air quality modelling applications

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TFEIP 2026 Meeting (Copenhagen, 11-13 May 2026)

Spanish Emissions Inventory System

INFORMATIVE INVENTORY REPORT
AIR POLLUTANTS

SUBMISSION TO THE SECRETARIAT OF THE UNECE
CONVENTION ON LONG-RANGE TRANSBOUNDARY AIR
POLLUTION AND TO THE EUROPEAN UNION UNDER
DIRECTIVE (EU) 2016/2284



Fulfil air quality modelling input requirements
(gridded, vertical, temporal, speciated)

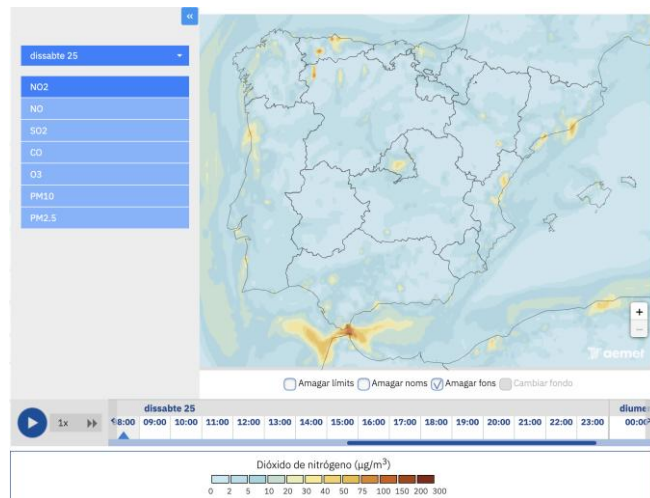


HERMES_Δ



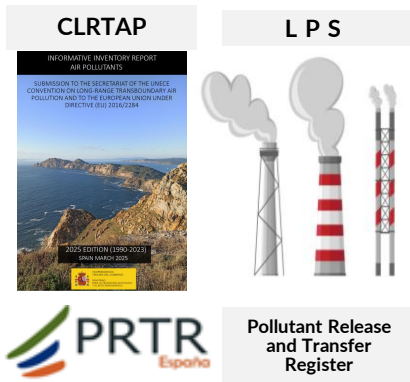
Provide feedback to inventory compilers
(modelled versus observed concentration)

AEMET national air quality forecast



HERMES_Δ: High-Elective Resolution Modelling Emission System, version Delta

Official inventories



- NUTS-2 & facility level
- Refined SNAP/NFR* sectorial classification (~ 630 emission sources)
- NO_x, NMVOC, SO_x, CO, NH₃, PM₁₀, PM_{2.5}, BC, BaP

Proxies & profiles

- **Horizontal:** ~140 spatial proxies
- **Temporal:** ~650 monthly, weekly and hourly profiles
- **Vertical:** stack height and sector-dependent vertical profiles
- **Speciation:** splitting NMVOC, NO_x and PM_{2.5} into chemical mechanism species

Ready-to-use emissions for modelling

Compatible with MONARCH, CHIMERE, MOCAGE, CMAQ, WRF-CHEM 3D air quality models + R-LINE gaussian model

Iberian Peninsula



Canary Islands



(*) Shipping, other countries and forest fires: processing of CAMS emissions using HERMES_GR (Guevara et al., 2019)

Spatial mapping

Processing of the LPS and PRTR-Spain official point source databases:

- Review of the original geographical coordinates (feedback to MITECO)
- Assignment of SNAP/NFR code to each PRTR-Spain facility (via Integrated Environmental Authorizations)
- Gapfilling of missing PRTR-Spain emissions (pollutants below information threshold)
- Remove duplicates between LPS y PRTR-Spain (giving preference to LPS)

Share of total GNFR_A + GNFR_B emissions directly allocated to specific industrial facilities

	NO _x	PM _{2.5}
EMEP	69%	23%
HERMES_Δ	94%	69%

EMEP: LPS

HERMES_Δ : LPS+PRTR+in-house point source catalogue

LPS+PRTR-Spain NO_x (2023)



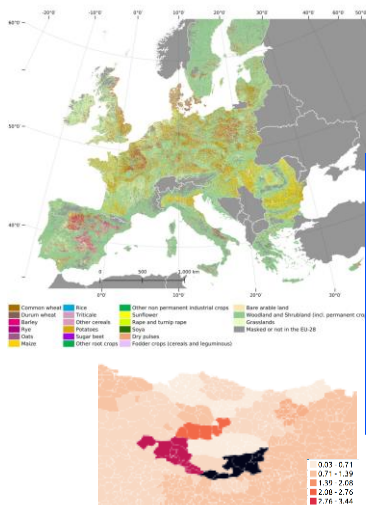
Spatial mapping

- Building on state-of-the-art global and European + national (existing and in-house) georeferenced proxies
- HERMES_Δ allows a flexible mapping to multiple:
 - Projections (regular lat-lon, rotated lat-lon, lambert conformal conic)
 - Resolutions (recommended up to 1km + link-level for road transport emissions)

Global-EU proxies

EUCROPMAP

21 crop types at 10m



GHSL

Population density & urbanisation degree (1km)

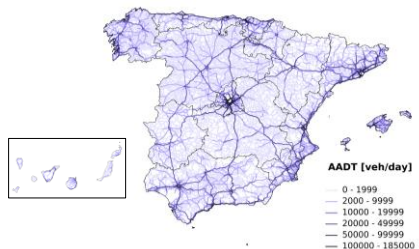


Households using biomass as main domestic heating fuel

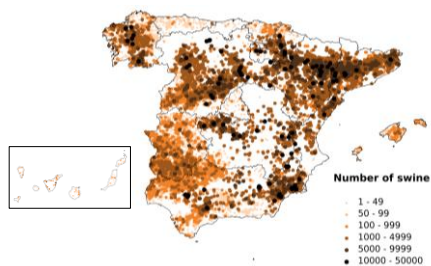


National existing proxies

Interurban & rural road network (AADT)



REGA Farms (n° animals)



National in-house proxies

Biogas plants



District heating plants



Fuel storage



Composting plants



Vertical distribution

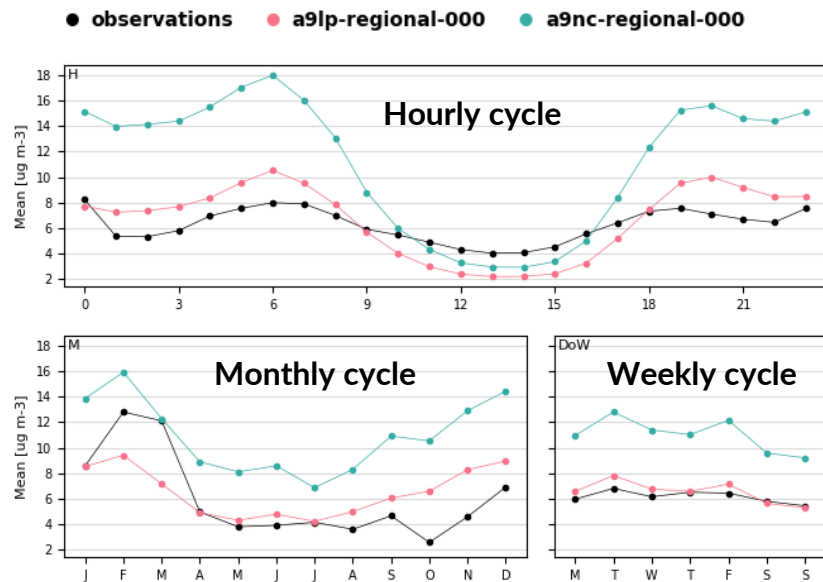
- **Point sources:** stack height¹ × plume rise factor²
- **Diffuse sources:** vertical profiles from literature
 - Guevara et al. (2020) for LTO cycles in airports
 - Bieser et al. (2011) for industrial diffuse sources
 - Grythe et al. (2019) for residential combustion



¹ Facility-dependent

² Based on Pregger and Friederich (2009)

NO₂ mod vs obs levels (ES1755A, 2023)

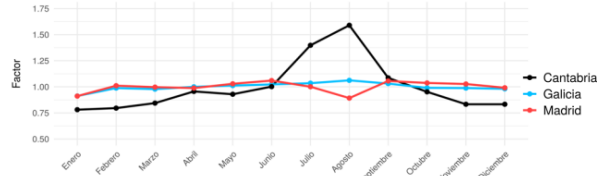


Temporal distribution

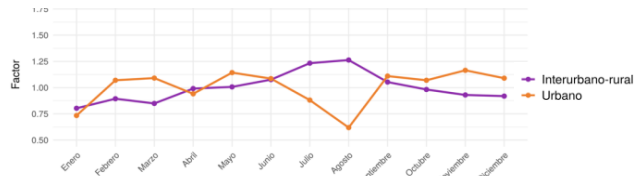
Original annual emissions broken down into hourly resolution

- Use of NUTS2 and sector-dependent monthly/weekly/hourly profiles to represent sociodemographic & climatological influences
- Possibility of using day-of-the-year profiles (e.g., based on heating degree days for residential combustion emissions)
- Automatic identification of **national** and **regional** holidays (treated as Sunday day type)

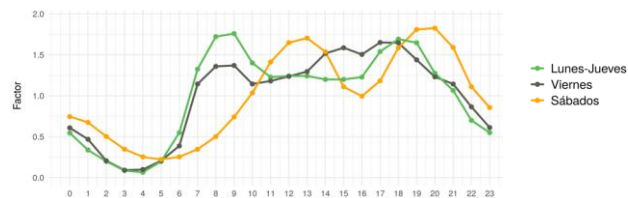
NUTS2-dependent monthly interurban profiles



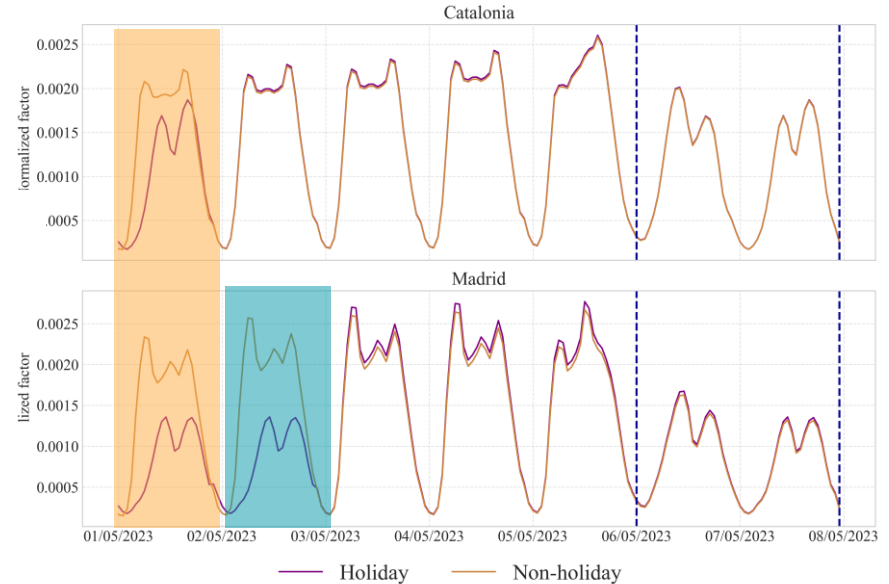
Interurban versus urban monthly profiles (Valencia)



DoW-dependent urban hourly profiles (Catalonia)



Hourly temporal weight factors for road transport



Speciation

A flexible two-step approach to go from reported pollutants to chemical mechanism species

Reported emission pollutants

- NMVOC
- NO_x
- PM_{2.5}

1. Split to individual chemical species

- Nitrogen monoxide
- Nitrogen dioxide
- Black carbon
- Organic carbon
- Ethylbenzene
- Toluene
- Benzene
- n-butane
- ... (> 800 species)

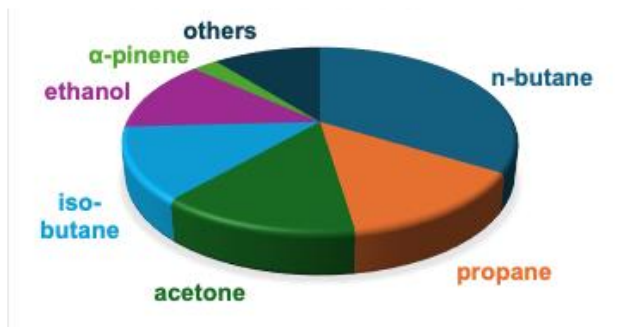
2. Mapping to chemical mechanism species

- Carbon Bond 5 & 6
- MELCHIOR
- CRACMM 1 & 2
- RACM
- explicit

Use of mapping tables (e.g., Carter et al., 2010)

Possibility to add additional chemical mechanisms

NMVOC split: Domestic use of solvents

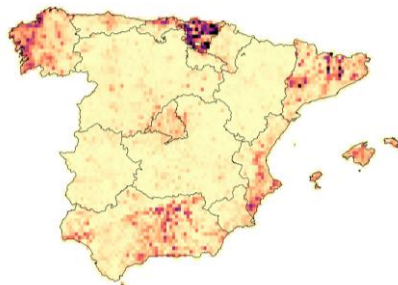


Use of ~150 sector-dependent NMVOC speciation profiles (Oliveira et al., 2025)

Comparison against state-of-the-art bottom-up and satellite-based inventories

GNFR C (Other stationary combustion) – PM_{2.5}

HERMES_Δ

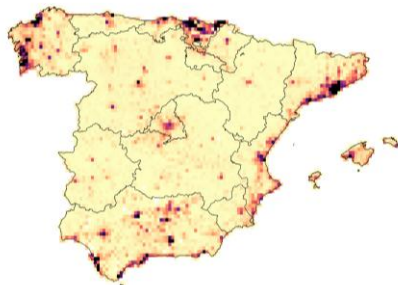


[t/year-cell]



GNFR C (Other stationary combustion) – PM_{2.5}

EMEP

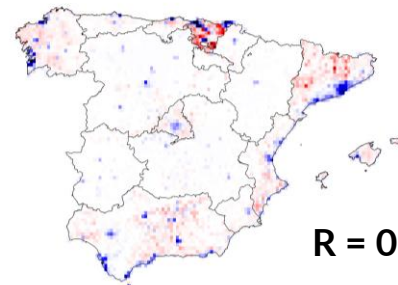


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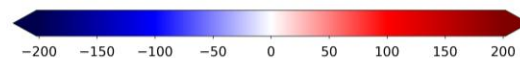


GNFR C (Other stationary combustion) – PM_{2.5}

HERMES_Δ - EMEP

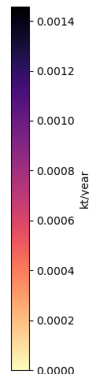
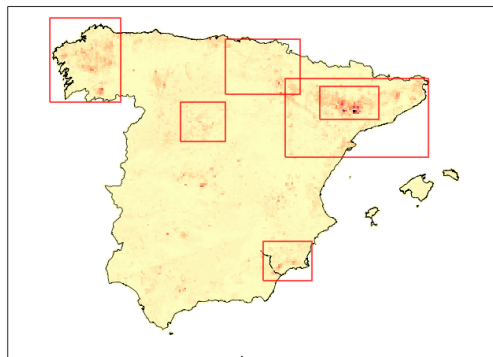


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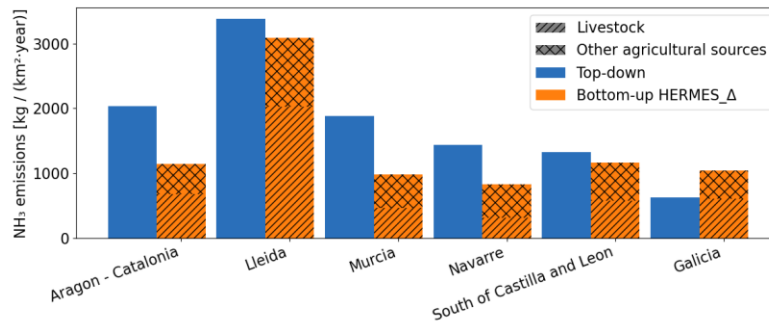


R = 0.32

HERMES_Δ: NH₃ annual emissions



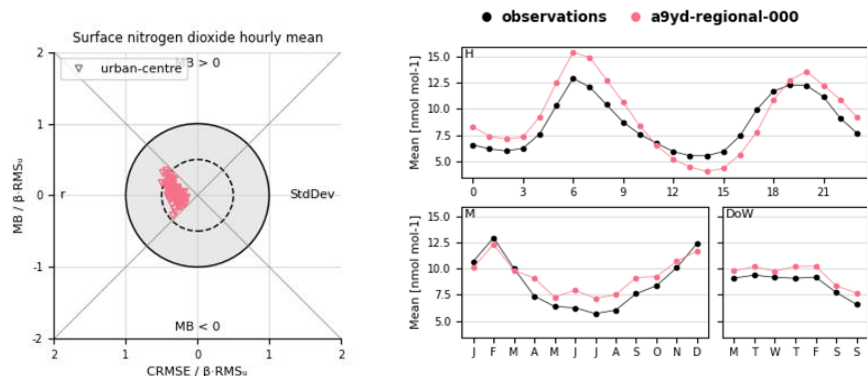
IASI NH₃ vs HERMES_Δ by region (normalized per area)



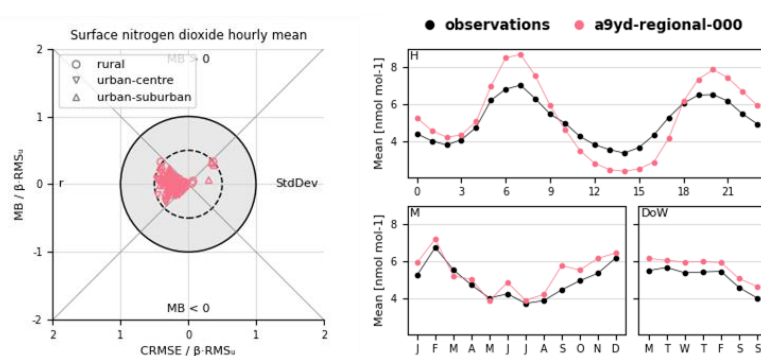
Indirect evaluation using air quality models and observations

NO₂

Urban background stations (n = 75)

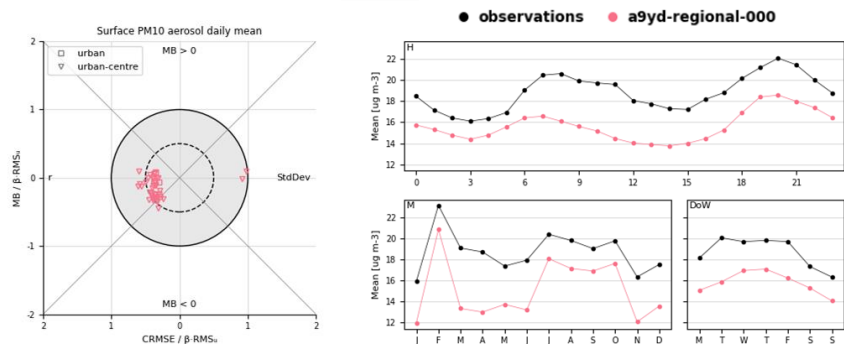


Industrial stations n = 122

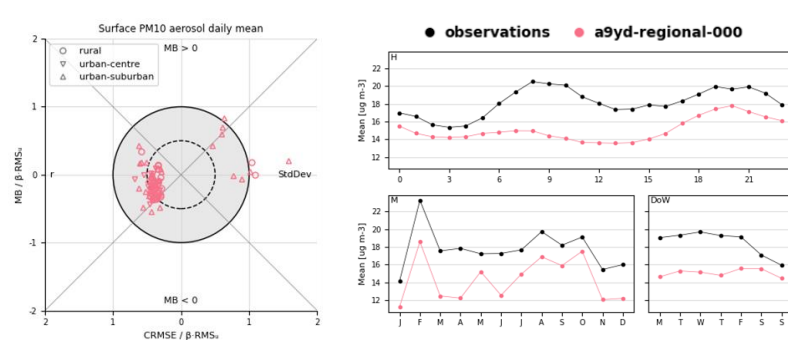


PM₁₀

Urban background stations (n = 50)



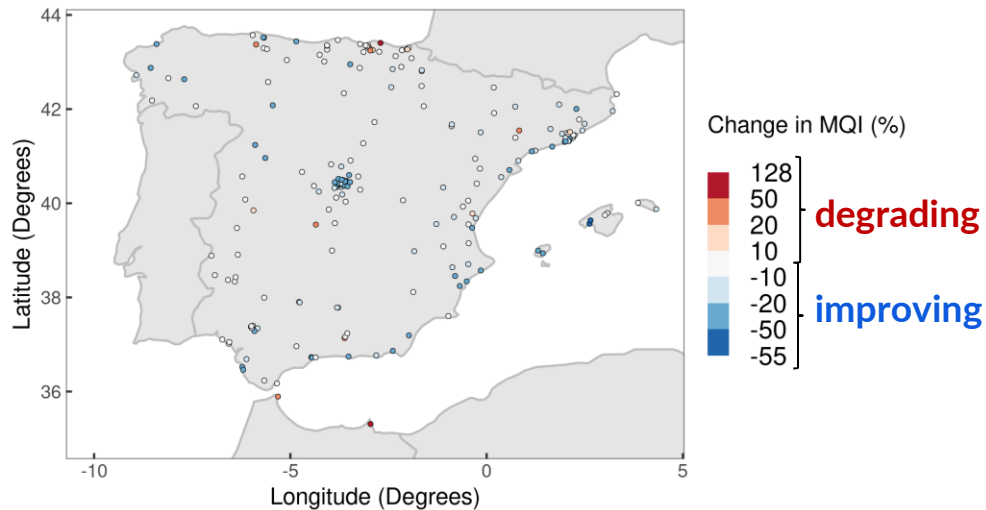
Industrial stations (n = 100)



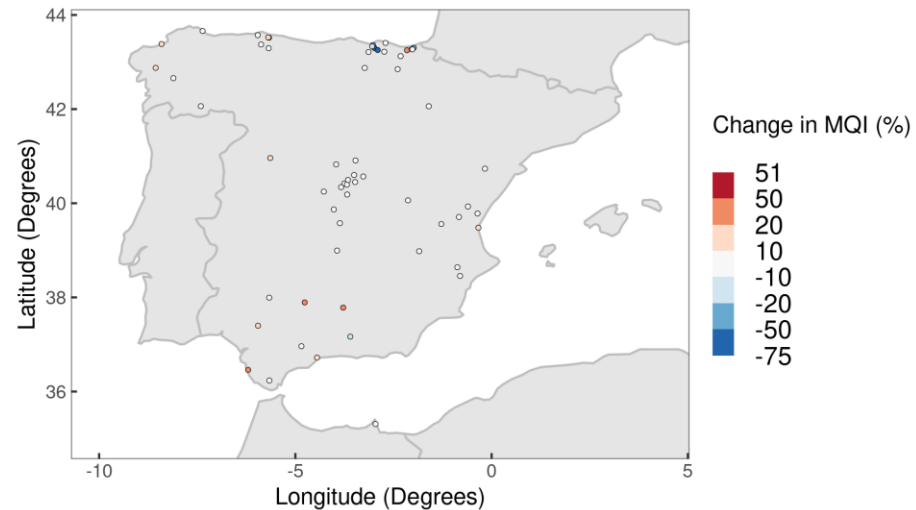
Indirect evaluation using air quality models and observations

Is the performance of the model improving or degrading when compared to the use of the EMEP inventory?

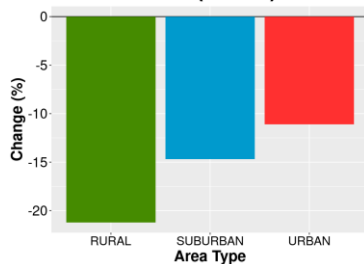
NO₂ (Mean1h)



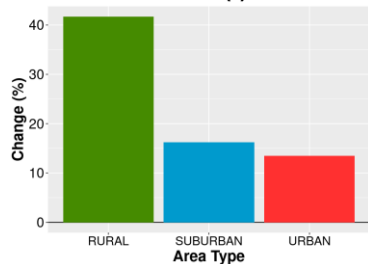
PM_{2.5} (Mean24h)



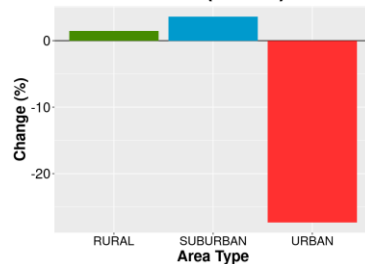
NO₂ (RMSE)



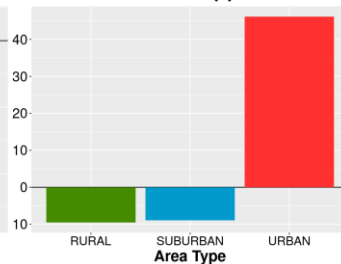
NO₂ (r)



PM_{2.5} (RMSE)



PM_{2.5} (r)



Courtesy of M. Theobald

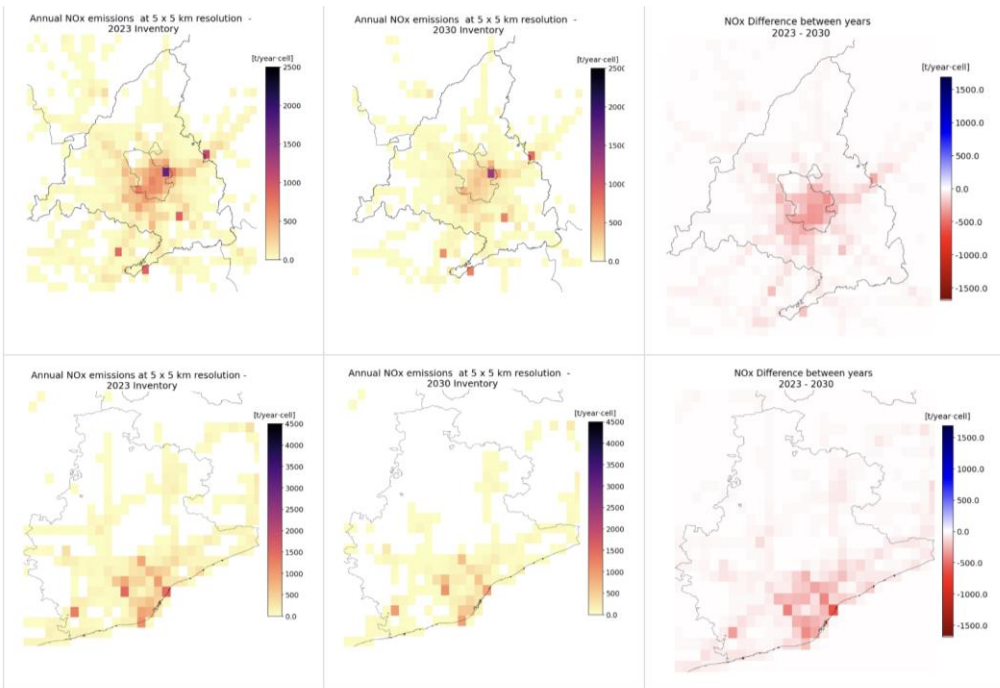
Support modelling efforts for air quality planning purposes

Flexible framework to prepare future emission scenarios consistent with official projections

2023 baseline

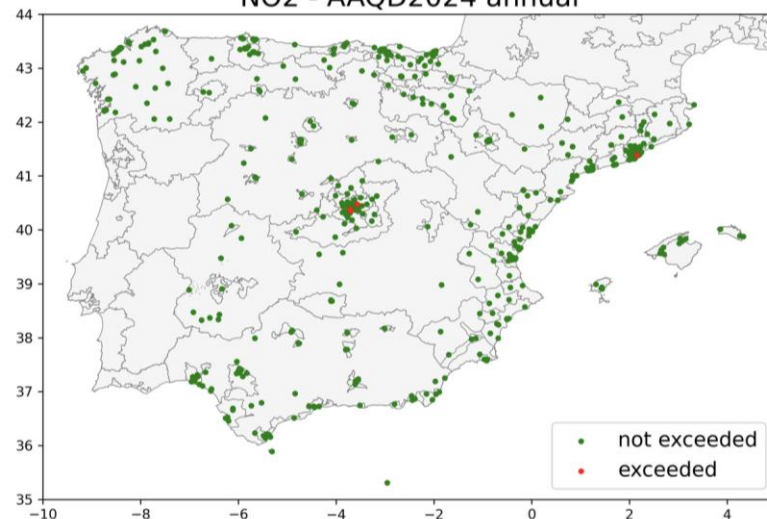
2030 WaM

Differences



2030 air quality scenario

NO2 - AAQD2024 annual



Take home messages

- Generation of **robust emission data** to support air quality modelling applications in line with the European Air Quality Directive 2024/2881:
 - Emission core of the national & Catalan air quality forecast systems (pre-operational mode)
 - Input to modelling exercises to support preparation of 2028-2035 air quality road maps
- Facilitate a **two way communication** between national inventory agencies and air quality modellers ("win-win": receive the most refined emission data + provide feedback & QA)
- Effort to **collect, integrate and process** multiple EU, national and subnational proxies and profiles to accurately reflect key spatio-temporal and speciation aspects of emissions
- In line with other efforts and initiatives:
 - At the national level: Germany ([GRETA](#)), US ([SMOKE](#))
 - At the EU level: TFEIP guidance for emission inventory users
- HERMES_Δ software in **open access** ([Tena et al., 2026](#)) – scientific paper under preparation
- **Next steps:** continue validation works and refinement of proxies + addition of missing sources (road dust resuspension)

Thanks for your attention!

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The project is part of the Recovery, Transformation and Resilience Plan (Plan de Recuperación, Transformación y Resiliencia, PRTyR) funded by the European Commission – NextGenerationEU.

The authors would like to acknowledge J. Pérez-Illzarbe, C. Ramos and the National Inventory team from MITECO for the information provided on the emission inventory and their feedback on the analysis of the results