Estimation of NOx emissions from point sources in Spain using TROPOMI observations and lightweight inversion methods

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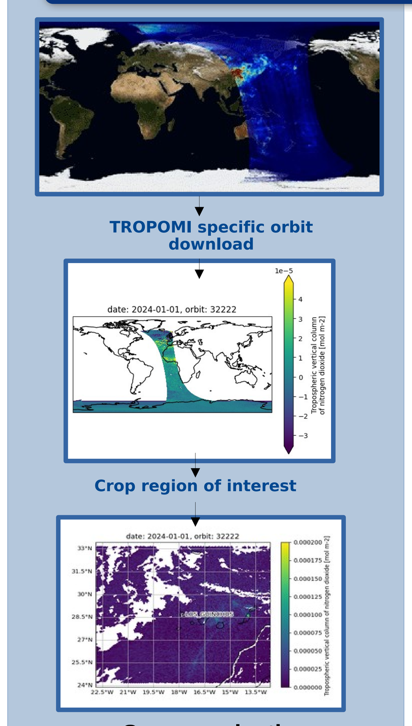
Introduction (WHY)

To comply with global emission reduction commitments, accurate monitoring and estimation of pollutant emissions are essential. **Nitrogen oxides (NO_x)** are gaseous compounds composed mainly of nitrogen and oxygen, predominantly produced during combustion processes. In **Spain**, key anthropogenic **point-source emitters** of NO_x include power plants, cement facilities, petrochemical complexes, steel mills, and refineries. Traditional **satellite-based top-down emission estimation techniques** rely on computationally demanding inversions using Chemical Transport Models (CTMs) with data assimilation. The capability of satellites to measure atmospheric pollutant concentrations has improved considerably over the years, both in terms of spatial and temporal resolution which has facilitated the implementation of top-down emission estimation techniques. Recent **lightweight inversion methods** enable daily emissions estimation from individual sources using satellite observations, such as the NO_2 columns from the Tropospheric Monitoring Instrument (**TROPOMI**) onboard the **Sentinel-5 Precursor satellite** and wind fields from **ERA5**. This study applies the four lightweight methods—**Gaussian Plume (GP)**, **Integrated Mass Enhancement (IME)**, **Cross Sectional Flux (CSF)**, and **Lightweight Cross Sectional Flux (LCSF)**—implemented in the Python library ***ddeq* V1.0**, to estimate NO_x emissions from the major point sources across the peninsular and the insular Spain. These estimates incorporate dynamic **NO_x lifetimes** derived from **CAMS EAC4** reanalysis data and specific assumptions regarding the NO_x/NO_2 ratio, **effective wind fields**, source location, and emission injection characteristics. Emission results from these methods were compared to those obtained with the **HERMES_Δ** emission model, demonstrating their potential for timely monitoring of pollutant emissions.

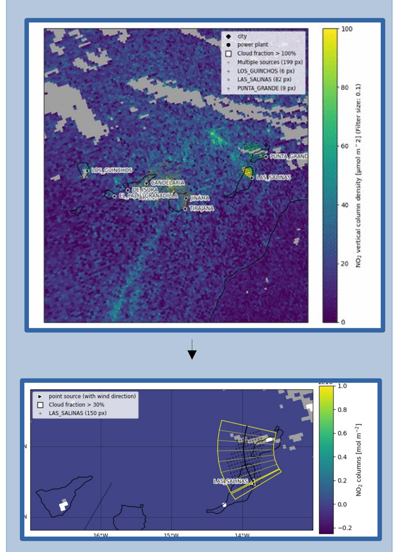
Methodology: (HOW)

Pipeline procedure used by the **ddeq 1.0 library** to estimate emissions from satellite data. The process is divided into four sequential stages



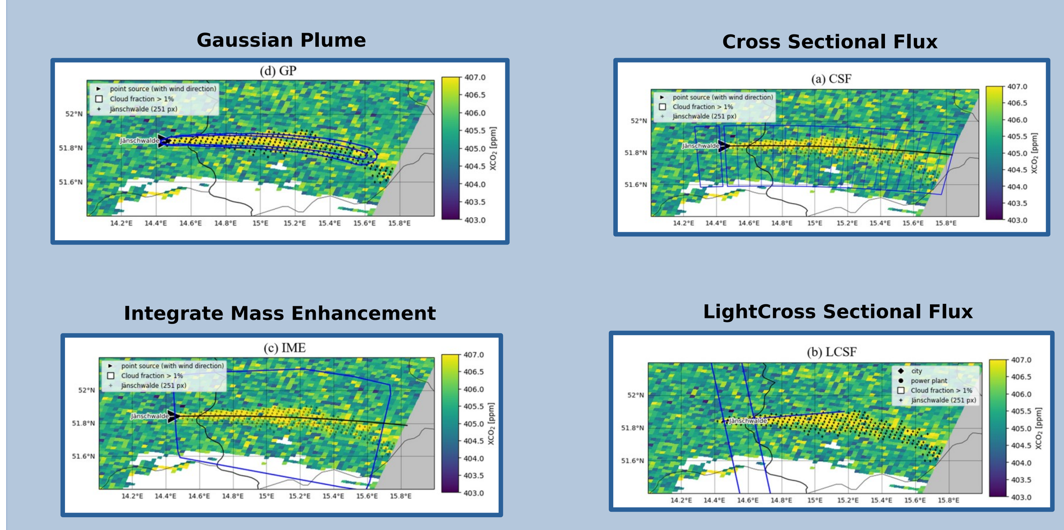
Source selection

1



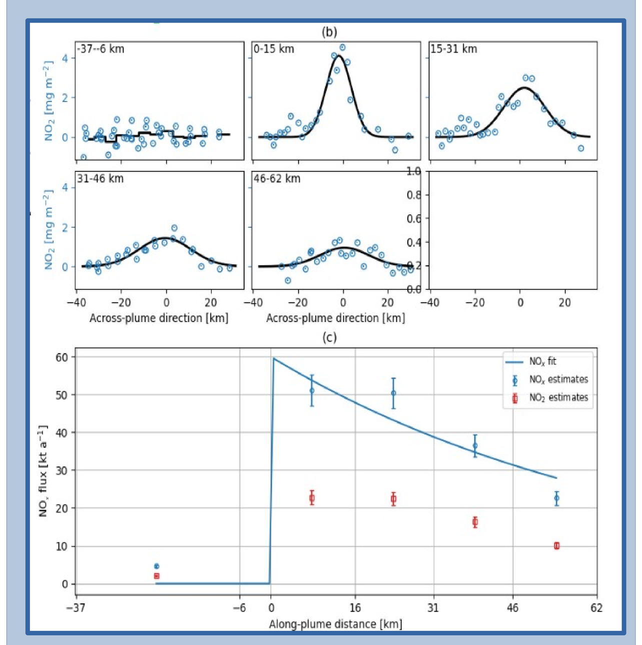
Plume detection

2



Lightweight emission estimation methods

3



Visualization

4

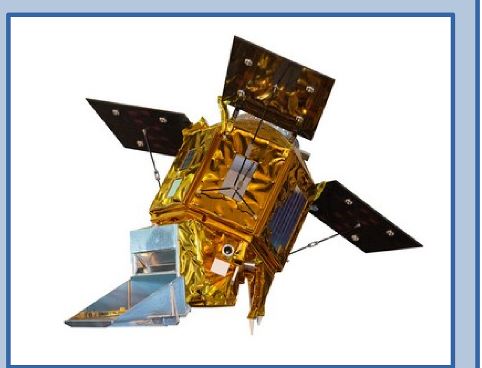
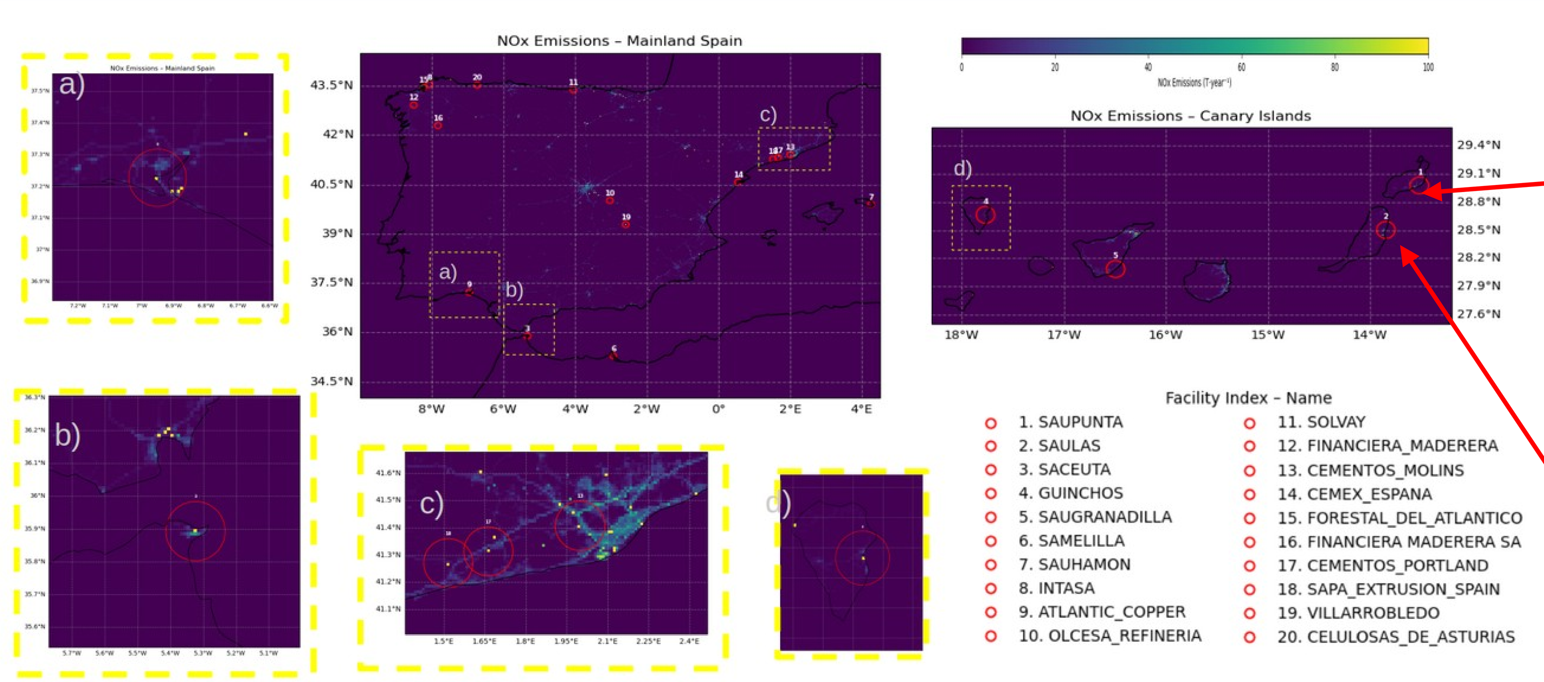


Fig 2: Sentinel 5 Precursor satellite with the (Tropospheric Monitoring Instrument) TROPOMI Instrument



Punta Piedra

Photo from Manolo de la Hoz (CC-BY-SA)

Las Salinas

Photo from Andy Mitchell from Glasgow UK(CC-BY-SA)

Fig 3: Selection of the Isolated top 20 emitters in the simulated emissions for 2021 from the HERMES_Δ model (project RESPIRE AIR https://respire.bsc.es/)

Results: (WHAT)

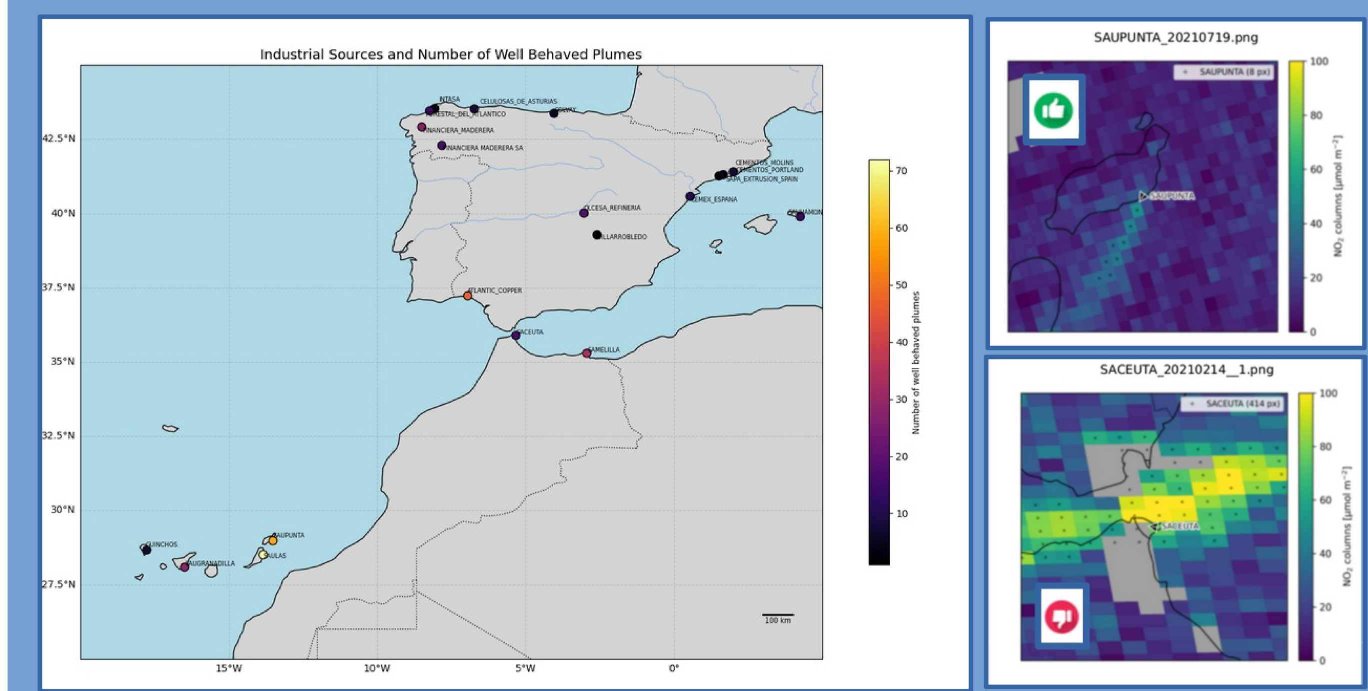


Fig 4: left Number of "good plumes" for 2021 for the Spain insular and peninsular domain and right an example of good and bad plume

Lifetime sensitivity experiments

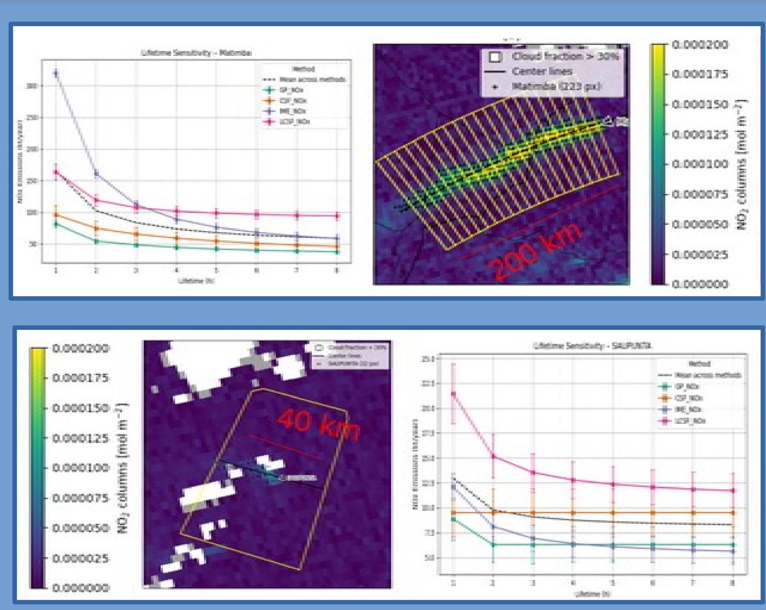


Fig 5: Lifetime sensitivity analysis for a high emission plume (Matimba) vs low emission plume (Saupunta- Canary Islands)

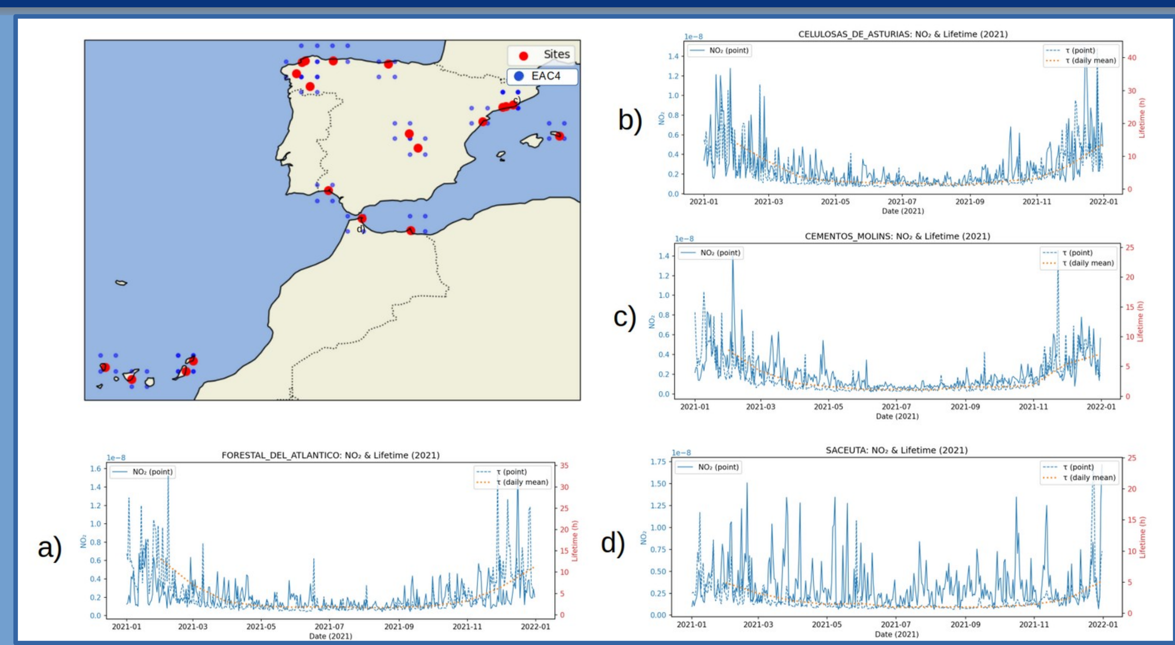


Fig 6: Top 20 industrial NO emitters in Spain, shown in red. In blue, the nearest grid points from the CAMS model corresponding to eachsource are marked. Panels (a) to (d) present time series of surface NO2 concentrations to estimated corresponding lifetimes,

NO2 lifetimes calculated using OH and temperature fields, lifetimes values go from the expected **10-15 hours in winter** to **1-4 hours in summer**

WHAT CAN BE CONSIDERED AS A "GOOD PLUME"?

- Pixel detected can be associated to a point source
- At least 4 pixels detected
- Not pixel detected behind the wind direction
- Wind direction of the model at least in the quadrants toward the wind direction
- Plumes without overlap of concentration from different sources.
- No data at all due cloud filtering or interrupted plume

Fig 7: Time series comparison for the Gaussian Plume (GP), Cross Sectional Flux (CSF), Integrated Mass Enhancement (IME) and Lightweight Cross Sectional Flux (LCSF) for two of the top 20 SPAIN high emitter with the HERMES_Δ. Case 1 corresponds to the use of static lifetime and Case 2 corresponds to the use of CAMS derived lifetimes

The Spanish NO_2 top emitters are low emission emmiters (<15Kt/y), compared with the high emissor emitters (30Kt/y<) for which the Lightweight methods have been tested before. The results suggest that Lower emissions present problems of plume detectability and quick dilution due to high wind regimes and ozone titration. (go to QR Supplementary material to see more results)

Discussions (SO WHAT)

USA experiment

Fig 6: Location of the Intermountain Power Plant, which is located in the heart of Utah, in Millard County. The right image shows the emissions values measured at the power plant stack

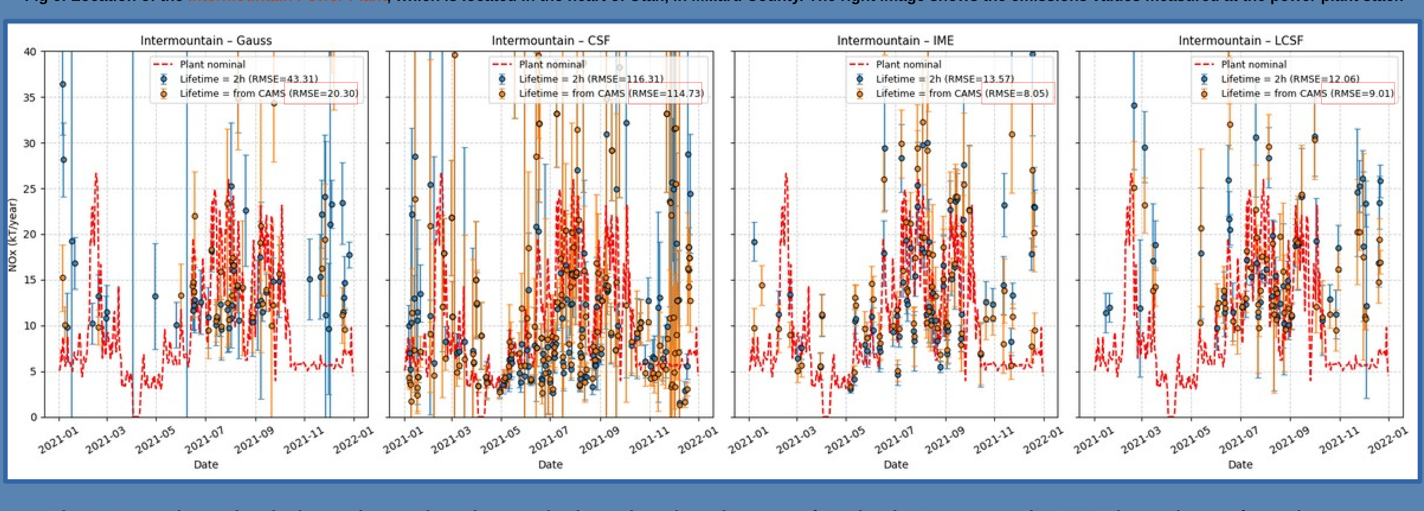


Fig 8: Comparison of emission estimates from four methods against the reference values for the Intermountain. RMSE is used to evaluate the performance of the methods against the emission reported from the power plant

Conclusions

Lightweight NO_x emission estimation techniques have proven effective for strong emission sources. Nevertheless, in scenarios characterised by low emissions – for example, the present low-NO_x context of Spanish power generation – these methods demonstrate diminished accuracy and robustness. *the "lighter" the plume, the heavier the challenge for the lightweight satellite methods*

It is crucial to enhance the plume detection process, as the presence of points that do not correspond to plumes can compromise the integrity of statistical analysis by introducing erroneous data.

Sources located near the coast are strongly affected by maritime traffic emissions or see breeze wind turbulent patterns. The overlapping transport patterns introduce Significant uncertainity, as individual plumes become difficult to distinguish from background maritime signals. This in general is not a good scenario for the *ddeq* methodology

In the context of the Intermountain scenario, which is regarded as the ideal case, the enhancement of the parametrization of lifetime has been shown to result in an improvement in the performance of all methods.

It is difficult to reach a definitive conclusion regarding the 20 top emitters in Spain; however, there is a tendency for improvement. In such instances, the lightweight methods encounter difficulties in producing estimations, owing to the presence of non-ideal cases, characterised by their non-isolated and non-high emitter status.

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supplementary material