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Detecting nitrogen oxide emissions in Qatar and quantifying emission factors of gas-fired power plants – a 4-year study

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1. Annual differences in horizontal distribution of NO_x emissions

The TROPOMI data used for NO_x emissions estimates were not all taken from the same version. Up to October 2021 included, we use the reprocessed S5P-PAL data (Eskes et al., 2021). This reprocessing provides a single consistent Sentinel-5P (S5P) TROPOMI NO_2 product (processed with same processor – version 2.3.1). The dataset has been generated to allow consistent data analysis (e.g. trends in COVID-19 impact on air pollution) over the period 01/05/2018-14/11/2021. For the remaining period (from November 2021 to December 2022), we use the offline stream (OFFL), with processor versions 2.3.1 from November 2021 to October 2022 included, and 2.4.0 from November 2022. As a result, the emissions displayed in Figure 6 use heterogeneous TROPOMI data. To observe the impact of these version changes on the spatial distribution of emissions, the emissions of the four years concerned are displayed in Figure S1. The main difference that is observed is in the transport term, which is lower in absolute value in 2022 in the main emitting areas. The "dipole" shape that is obtained around the main emitters, i.e. Dammam (Saudi Arabia), Manama (Bahrain), Doha (Qatar), Ras Laffan (Qatar) and the south-east of Qatar is less pronounced in 2022, without being compensated by a lower sink term. As a result, maps for 2019 to 2021 show small areas with slightly negative emissions. The study of the influence of the quality limit factor q_a aims to provide an explanation for these differences.

2. Wind threshold for image filtering

Pollution from Bahrain, which is usually transported to Qatar, can reach Doha during strong wind events. In such situations, the errors in ERA5 can alter the estimation of the transport term and thus the NO_x estimates. In our monthly and annual estimates of NO_x emissions, we remove days with high wind speeds in the Bahrain/Qatar direction, i.e. days for which the average wind over Bahrain and the marine area between the two countries has a speed higher than 30 $km.h^{-1}$ and an angle between -15° (E¼SE) and -75° (S¼SE). These thresholds have been chosen as a threshold because it corresponds to the minimal value for the wind module to reach the closest high emitters of Qatar. Manama and the cement plants in the east (angle ~ -75°) are separated by ~ 110 km. Manama and the Ras Laffan power plants (angle ~ -15°) are separated by ~ 105 km. With an mean annual lifetime of 3.5 hours (calculated according to Equation 2), the value of 30 $km.h^{-1}$ corresponds to the minimal wind speed that would allow NO_2 pollution from Bahrain to overlap emissions in Qatar. This threshold value would be increased if mean lifetimes values for spring, summer and fall seasons (3.1 h, 2.1 h and 3.2 h respectively for years 2019-2022) were used. However, higher lifetime values during winter (5.2 h, DJF value for 2019-2022), would lower the threshold the ~ 21 $km.h^{-1}$.

Using lower values for the wind speed threshold at 25 and 20 $km.h^{-1}$, we observed that discarded days are increased from 169 to 240 and 309 respectively. About half of the additional discarded days correspond to days between December and March included, for which 4.25 additional days are discarded on average. Lowering the threshold generally leads to a decrease in emissions. On average, this does not impact the value of main emissions: with a threshold of 20 $km.h^{-1}$, emissions are lowered by about -2.6% for 2019-

2022. The decrease is about -6.0% on average for months between December and March included. Months for which the absolute change is higher than 10% are January 2019 (-10.7%, 3 additional discarded days), December 2019 (-20.1%, 7 additional discarded days), February 2021 (-14.2%, 7 additional discarded days) and December 2022 (-10.7%, 3 additional discarded days). These large diminutions are mostly due to the fact that the additional discarded days included moments for which pixels above the cement plants and Doha were visible, increasing thus the number of pixels which are never observed during a month.

3. Influence of quality assurance value threshold

The quality assurance value q_a is related to the presence of clouds and aerosols. Within each pixel, it ranges from 0 (no data) to 1 (high-quality data), and it is recommended to use data with $q_a > 0.75$ for remote sensing analysis. Within the study area, seven areas, including four in Qatar, have particularly low values for this flag. As these areas include several hotspots in the region, the correct estimation of the corresponding daily emissions is prevented, which lowers the robustness of monthly and yearly averages. Table S1 which is analogous to Figure 7, displays, for different periods, the frequency with which each pixel has its insurance quality value exceeding the threshold of $q_{a,\mathrm{lim}} = 0.75$, compared to a threshold of $q_{a,\mathrm{lim}} = 0.70$. For this lower threshold, columns are kept for all the domain most of the time (with a fraction of observed days higher than 80 % for all pixels). Here, if the S5P-PAL reprocessed data (version 2.3.1) from January 2019 to November 2021 displays pixels for which the value of q_a frequently falls below 0.75, the use of the OFFL stream (version 2.3.1) from November 2021 to November 2022 is characterised by pixels for which the value of q_a falls below 0.75 less frequently. Furthemore, the last two months of 2022, calculated with the version 2.4.0 of the TROPOMI product (operational since July 2022), do not show any areas with particularly low quality flag values. The latest version of the user manual indicates that in this version, OMI and GOME-2 derived surface albedo climatologies in the NO_2 fitting window were replaced by a surface albedo climatology derived from TROPOMI observations. This new TROPOMI surface is consistently applied in the cloud fraction, the cloud pressure retrievals, and in the air-mass factor calculation. This seems to indicate that the low values for q_a for the older versions originated from the previous algorithms used to calculated parameters involved in the calculation of q_a.

Figure S2 shows the annual NO_x emissions at 13:30 LT over Qatar using a quality insurance threshold of $q_{a,\mathrm{lim}} = 0.75$ for years 2019, 2020, 2021 and 2022, while Figure S3 shows the corresponding emissions with a threshold of $q_{a,\mathrm{lim}} = 0.70$. The comparison between the two figures highlights differences in emissions where high frequencies of pixels with $q_{a,\mathrm{lim}} < 0.75$ were encounted. Because this phenomenon is less marked for 2022, the corresponding maps are very similar, while maps for years 2019, 2020 and 2021 show pixels with lower emissions above several hotspots when the threshold is set to 0.75. In particular, the pixels between the urban area of Doha and the south-eastern part of the country show negative or zero emissions on Figure S2 but not on Figure S3.

The proper use of quality flags and uncertainty information is critical for an accurate use of the S5P data. Taking all NO_2 retrievals with a q_a value larger than 0.7 add the good quality retrievals over clouds or aerosol layers, which are not sensitive to the NO_2 concentrations near the ground. They still contain useful information, but this should be carefully interpreted. Standard analyses that do not take this into account will provide flawed results. Results shown on Figure S2 and S3 are not intended to replace the results calculated with a threshold of 0.75, as these mix data of different nature.

4. Weekly cycle for NO_x emissions, NO_2 tropospheric column densities and OH concentration above urban and industrial areas

The weekly cycle for NO_x emissions displayed on Figure 8 can be analysed with respect to the different parameters involved in the calculation of emissions. Figure S4 displays the weekly cycle of NO_2 VCDs, OH concentrations and NO_x emissions over the whole country (internal mask), the Ras Laffan power plants (using the six pixels that are the closest to the power plants) and the urban area of Doha (urban pixels of the metropolitan area according to the SEDAC-GRUMP dataset) for the 2019-2022 period (at around 13:30 LT). The 4-year average is calculated without accounting for values lower than the 5^{th} percentile or higher than the 95^{th} percentile of the ensemble (as explained in Section 5.4), and the re-scaling of the emissions using the load curve is not performed.

OH concentrations do not vary much within the week: the observed trend in NO_x emissions is thus mainly driven by changes in tropospheric columns. Moreover, the observed "week-end effect" observed for the country is stronger over Greater Doha, and weaker over the Ras Laffan power plants. It can therefore be assumed that this effect is mainly due to a reduction of transport emissions on Fridays.

5. Power demand ratio and rescaling of emissions

We use power demand time series in Qatar to re-sacle the emissions inferred by our method at 13:30 to obtain mean monthly emissions in Qatar. The power demand dataset has been obtain by Bayram et al. (2018) using C-Sharp by visiting the webpage of the Gulf Cooperation Council Interconnection Authority (GCCIA) and searching for keywords related to demand data. The website publishes data for five Gulf states. The dataset covers the twelve-month period from February 2016 to January 2017 with a one-minute resolution. Data published on the GCCIA website is expected to be accurate. Here, although electricity consumption has increased in Qatar between 2016 and 2019-2022, we assume that this growth has been uniform across days and months. Under these conditions, the ratio between the electricity demand at 13:30 local time and the average electricity demand remains unchanged. The corresponding values for each month are given on Table S2.

6. Sectoral comparison with inventories

The two inventories that are studied here (EDGARv6.1 for year 2018 and CAMS-GLOB-ANT_v5.3 for years 2019 to 2022) provide gridded maps with a 0.1°×0.1° resolution. In Qatar, most NO_x emissions are concentrated winthin three sectors:

- **energy** (power industry, IPCC 1A1a)
- **transport** (shipping, aviation, and road transportation, IPCC 1A3a_CDS + 1A3a_LTO + 1A3d + 1C2 + 1A3a_CRS + 1A3b_noRES)
- **industry** (oil refineries and transformation industry, combustion for manufacturing, chemical processes, IPCC 2B + 1A2 + 1A1b + 1A1c + 1A5b1 + 1B1b + 1B2a5 + 1B2a6 + 1B2b5 + 2C1b).

Other sectors (agricultural soils, manure management, energy for buildings, fuel exploitation, solid waste incineration, agricultural waste burning, IPCC 4C + 4D + 4B + 1B1a + 1B2a1 + 1B2a2 + 1B2a3 + 1B2a4 + 1B2c + 4F + 1A4 + 6C) only represent a small part of the total NO_x budget. The output for each sector is represented on Figure S5 for EDGARv6.1 and on Figure S6 for CAMS-GLOB-ANT_v5.3. Because the resolution is different than what is used in our TROPOMI-inferred estimates of NO_x emissions (0.0625°×0.0625°), we use a 0.1°×0.1° mask which has a similar shape as the internal mask displayed on Figure 3. Although the seasonality and amplitude of emissions from the inventories differ from the emissions estimated by our model, their spatial distribution is similar. Power emissions are located in Doha, the south-east of Doha and in the Ras Laffan area. The industrial sites are mainly located in Doha, and we note the presence of an emissive pixel in the west of the country which could correspond to the cement plants previously identified. The transport emissions spreads from Doha to the peripheral areas (north, west and south-west). Figure S7 displays the map of NO_x emissions for those three sectors for EDGARv6.1. The corresponding map for CAMS-GLOB-ANT_v5.3 is very similar.

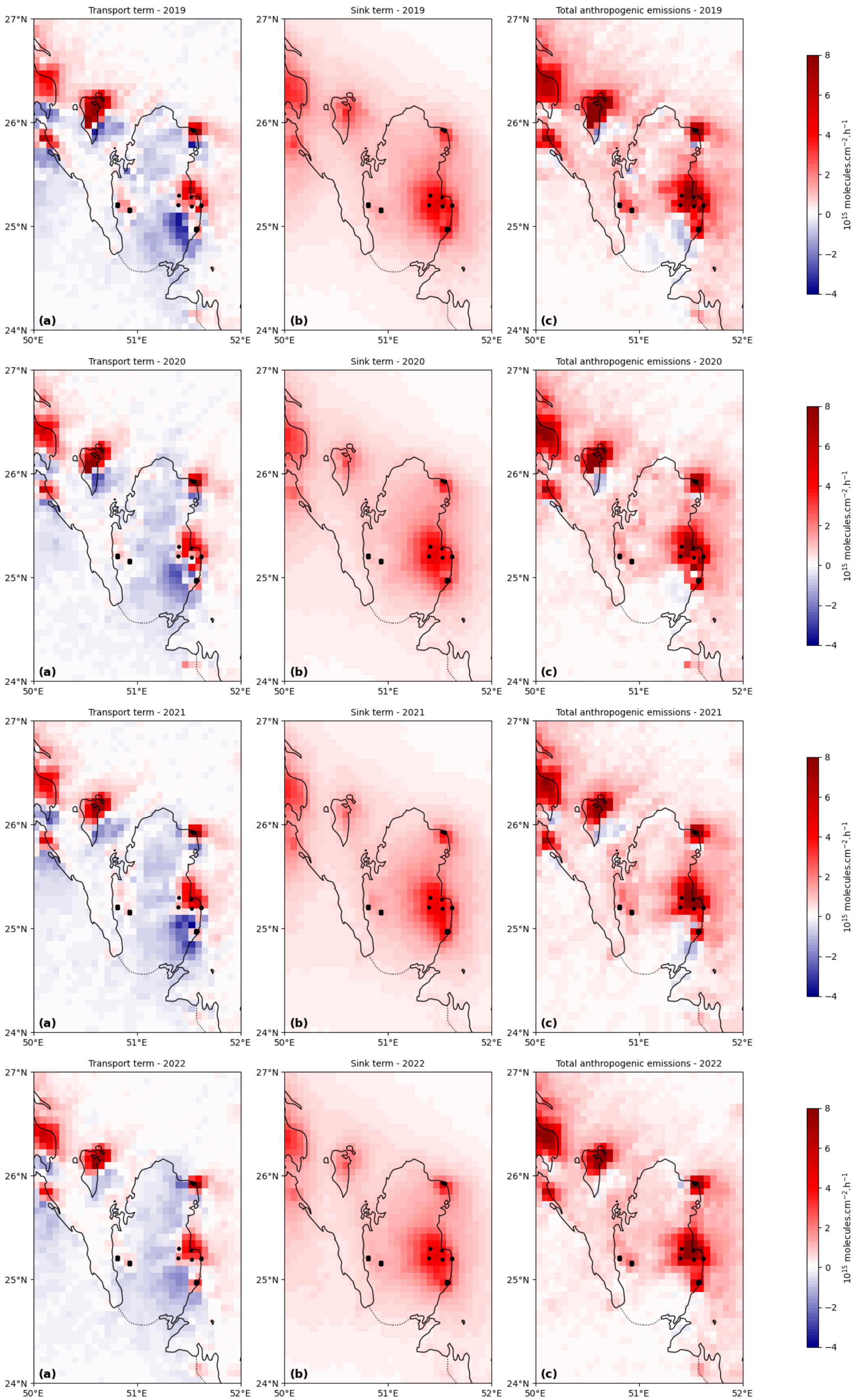
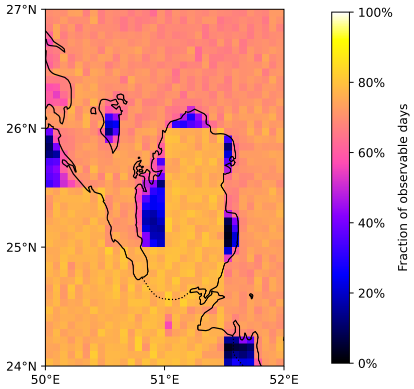
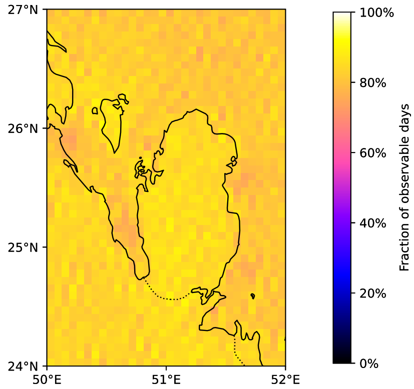
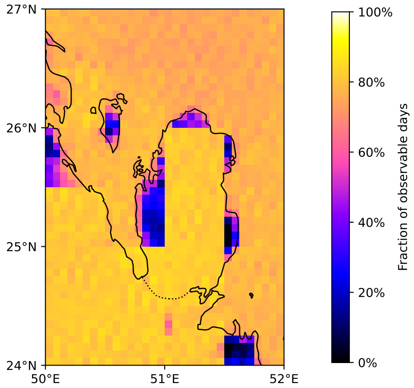
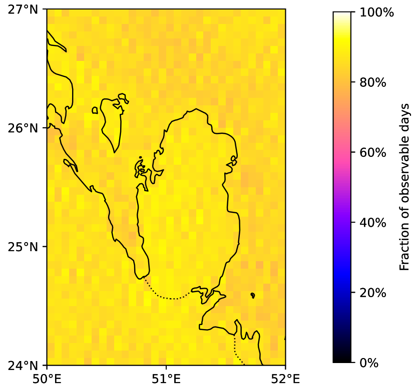
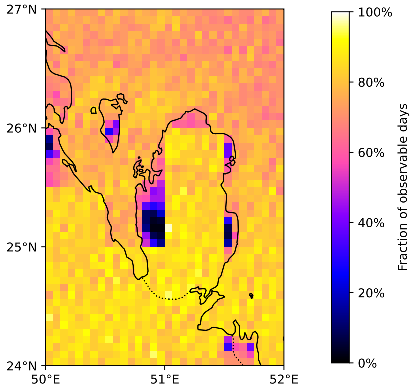
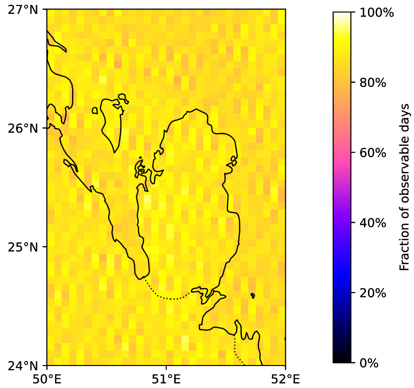
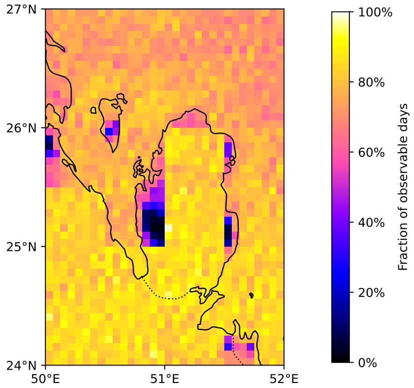
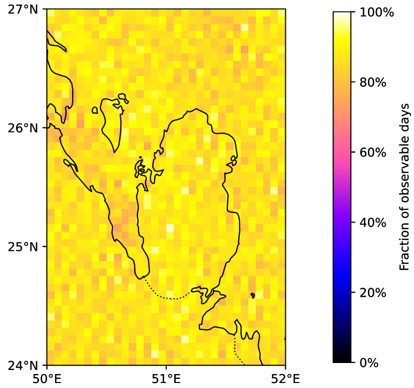


Figure S1: Mean NO_x emissions above Qatar (13:30 LT): transport term (a), sink term (b), and resulting emissions (c) for years 2019 to 2022 (top to bottom). Power plants are denoted with dots, cement plants with squares, and Doha with a star.

Period	**Data version**	$q_{a,lim}$ **= 0.75**	$q_{a,lim}$ **= 0.70**
2019	2.3.1 with S5P-PAL reprocessing		
2020	2.3.1 with S5P-PAL reprocessing		
2021	2.3.1 with S5P-PAL reprocessing from Jan. 2021 to Oct. 2021 included		
2021/11-2021/12	2.3.1		

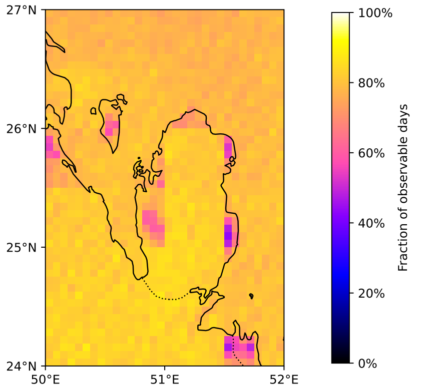
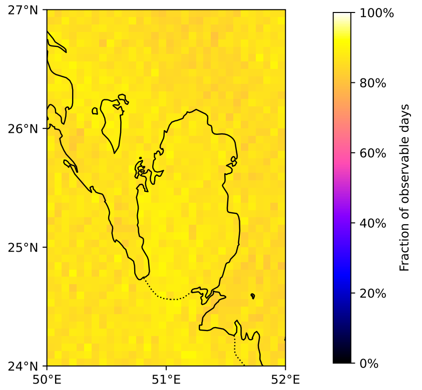
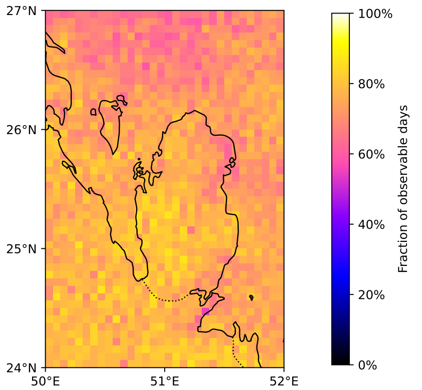
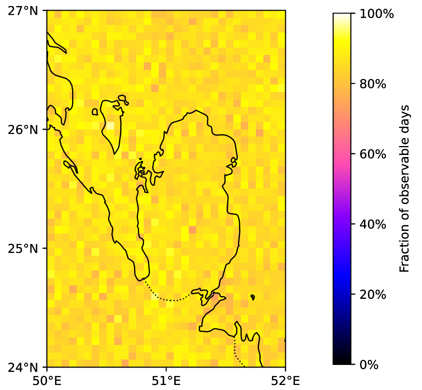
2022	2.3.1 from Jan. 2022 to Oct. 2022 included and 2.4.0 from Nov. 2021 to Dec. 2022 included.		
2022/11-2022/12	2.4.0		

Table S1: Comparison between TROPOMI observation densities for different periods between 2019 and 2022 with a quality threshold of $q_{a,lim}$ = 0.75 (left) and $q_{a,lim}$ = 0.70 (right). The corresponding TROPOMI version is indicated for each period.

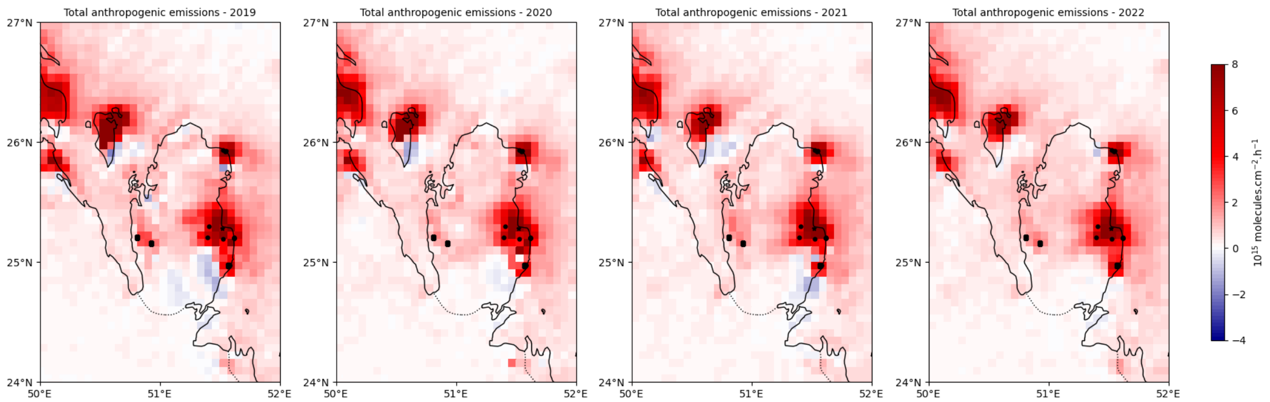


Figure S2: Annual mean emissions at 13:30 for years 2019 to 2022 (left to right) with quality flag threshold equal to q_a = 0.75.

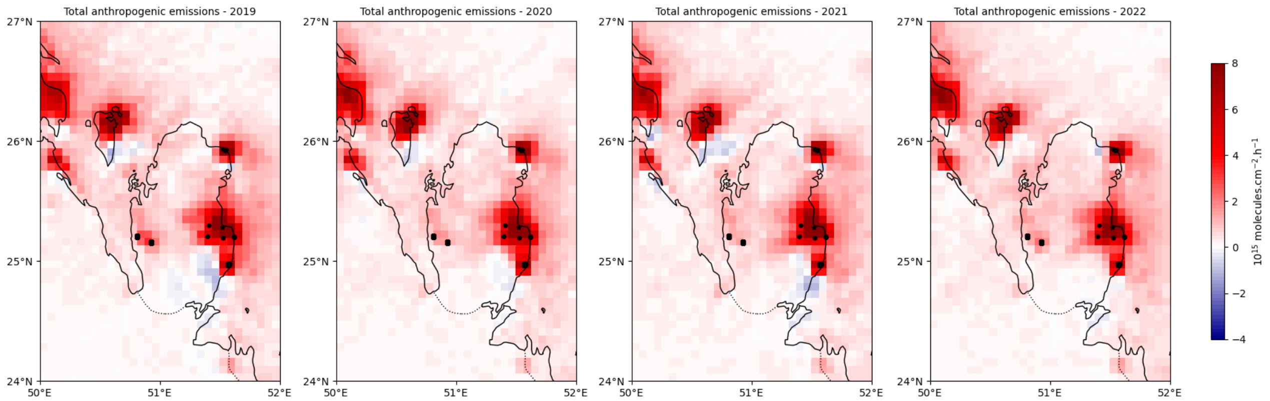


Figure S3: Annual mean emissions at 13:30 for years 2019 to 2022 (left to right) with quality flag threshold equal to q_a = 0.70.

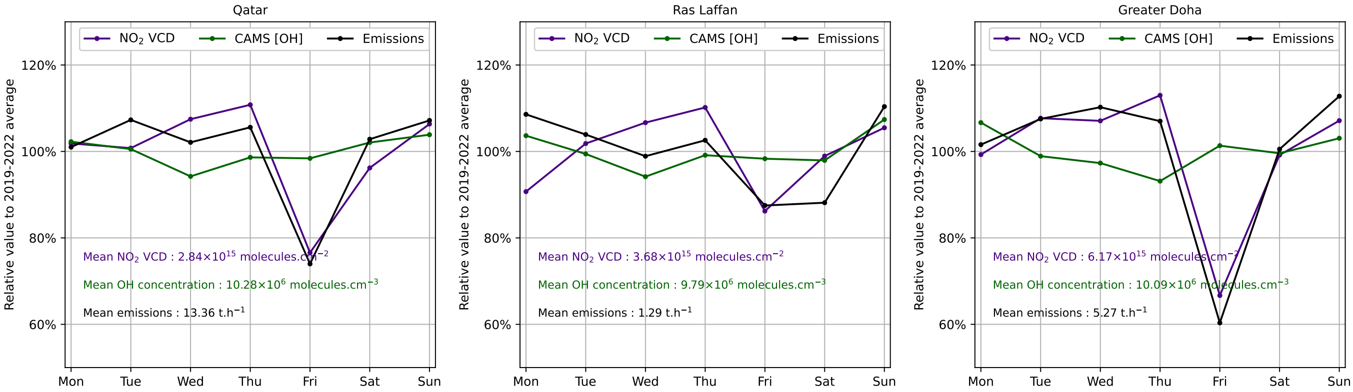


Figure S4: Mean weekly profiles for NO_2 tropospheric vertical columns, OH concentration and NO_x emissions for the entire country (left), the Ras Laffan power plants in the north (middle), and the Greater Doha area (right). The 2019-2022 average is given and represented by the 100% line.

Month	**Ratio $P_{13:30}/\langle P \rangle$**
January	0.967
February	0.976
March	0.965
April	0.932
May	0.914
June	0.911
July	0.918
August	0.922
September	0.921
October	0.924
November	0.944
December	0.960

Table S2: Ratio between mean daily power demand and power demand at 13:30, averaged for each month between February 2016 and January 2017 and expected to be valid from 2019 to 2022.

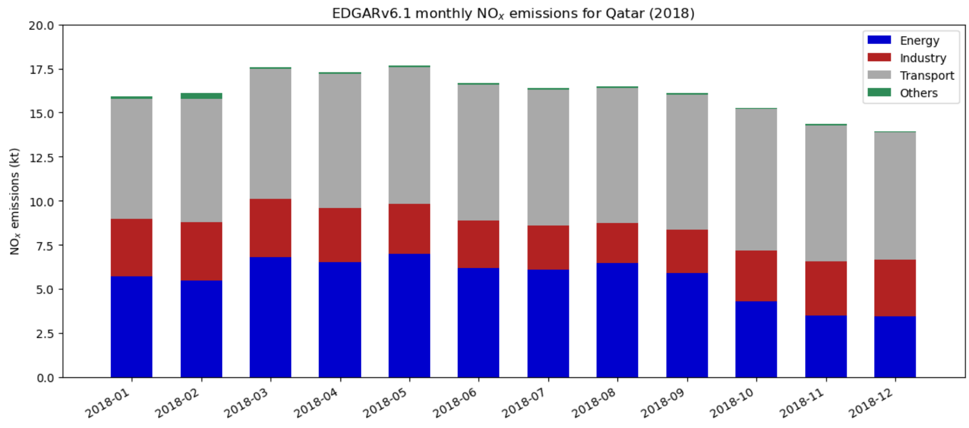


Figure S5: Monthly terrestrial NO_x emissions in Qatar for year 2018 in EDGARv6.1 by sector.

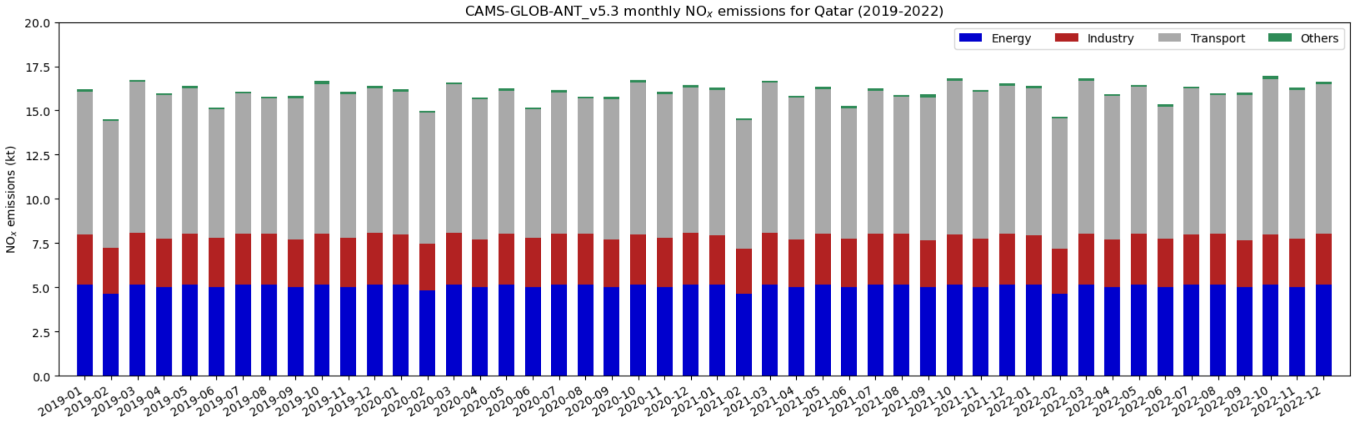


Figure S6: Monthly terrestrial NO_x emissions in Qatar for years 2019 to 2022 in CAMS-GLOB-ANT_v5.3 by sector.

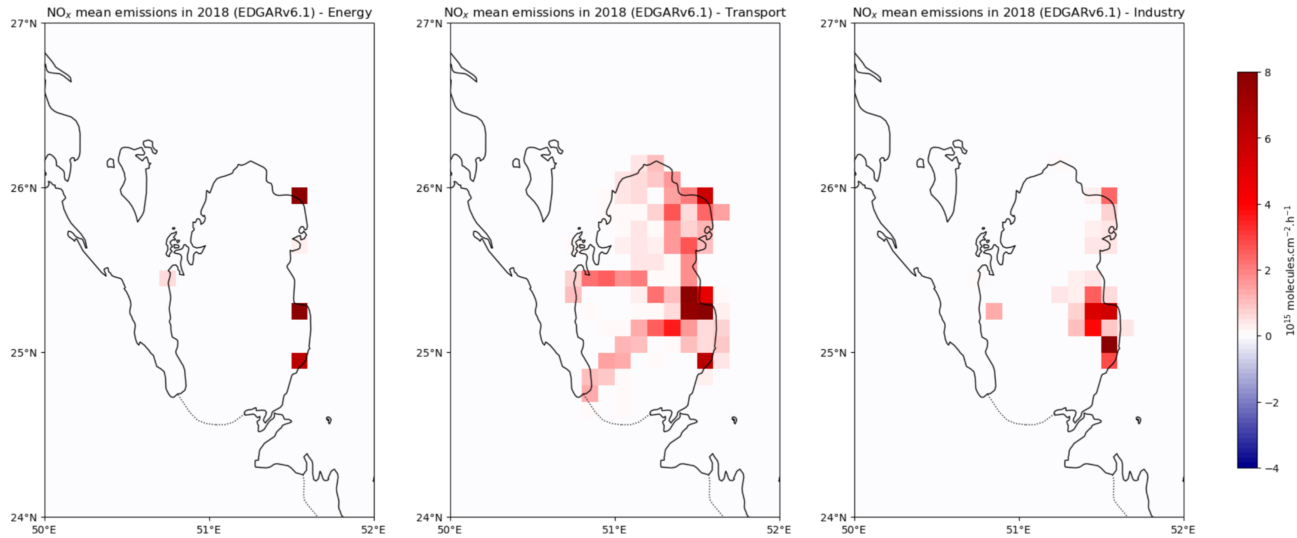


Figure S7: Map of annual NO_x emissions in Qatar for years for EDGARv6.1 within the internal mask for the power (left), transport (middle) and industry (right) sectors.

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