Electronic Supplementary Material (ESI) for Environmental Science: Atmospheres.

Supplemental Information for:

Local scale NO_2 impacts in the Los Angeles Basin from increased port activity during 2021 supply chain disruptions

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Port throughput data

Table S1. Total twenty-foot equivalent unit (TEU) throughput at the Ports of Los Angeles and Long Beach combined in 2018, 2019, and 2021.

	2018	2019	2018-2019 average	2021	2021 increase
January	1,466,559	1,509,736	1,488,147	1,599,522	7%
February	1,386,850	1,301,924	1,344,387	1,571,050	17%
March	1,153,124	1,203,798	1,178,461	1,797,986	53%
April	1,323,975	1,364,588	1,344,281	1,693,154	26%
May	1,456,231	1,402,286	1,429,259	1,919,264	34%
June	1,475,330	1,441,945	1,458,638	1,600,727	10%
July	1,522,026	1,533,935	1,527,981	1,675,645	10%
August	1,506,181	1,525,074	1,515,628	1,762,081	16%
September	1,502,469	1,486,858	1,494,663	1,652,337	11%
October	1,657,962	1,458,614	1,558,288	1,692,360	9%
November	1,454,165	1,328,902	1,391,533	1,556,948	12%
December	1,644,905	1,412,012	1,528,458	1,540,903	1%
Total Calendar Year	17,549,778	16,969,670	17,259,724	20,061,978	16%

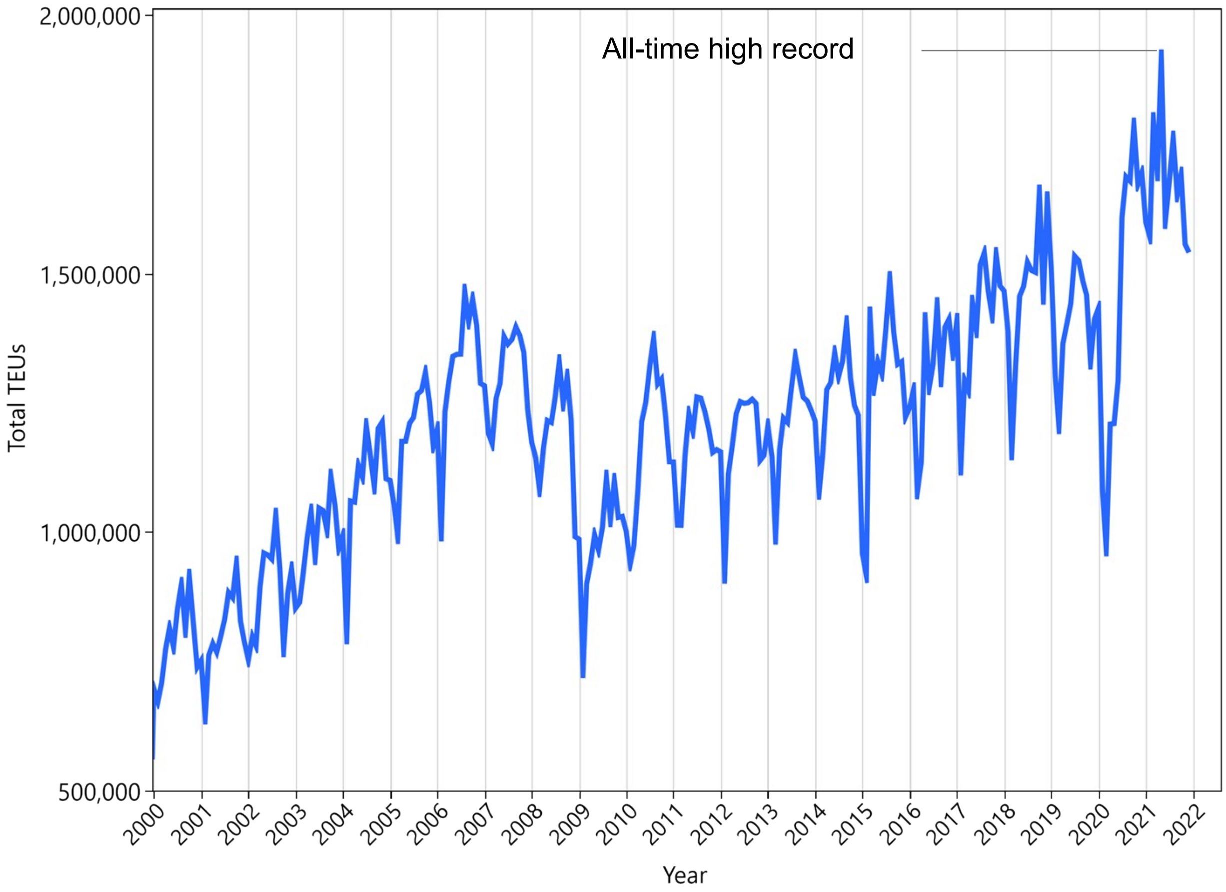

Figure S1. Monthly total TEUs (twenty-foot equivalent units) at Ports of Los Angeles and Long Beach from 2000-2021. TEU throughput reached an all-time high in 2021. TEU data sources:

https://www.portoflosangeles.org/business/statistics/container-statistics

https://polb.com/business/port-statistics/

Ships at anchor location

Figure S2. Image of ships near the Ports of Los Angeles and Long Beach captured by the Operational Land Imager (onboard Landsat 8) on October 10, 2021. Image obtained from https://earthobservatory.nasa.gov/images/149004/scientific-questions-arrive-in-ports.

CMAQ modeling domain

Figure S3. CMAQ modeling domain with a horizontal resolution of 4 km × 4 km.

CMAQ meteorological adjustment to NO_2

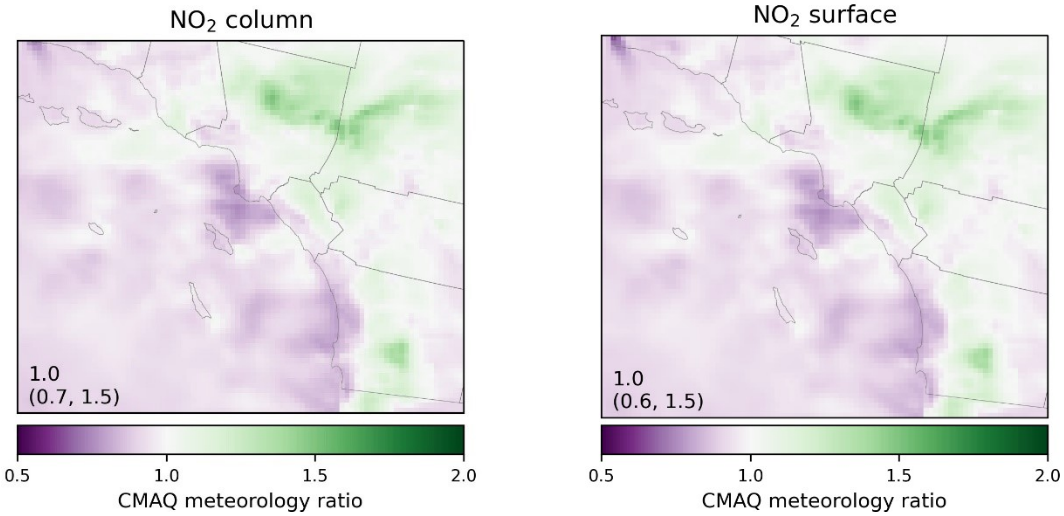

Figure S4. The CMAQ meteorology ratio described in Eq. 1 of the main text. The results shown here are for the average of September-November for 2018 and 2019 at the TROPOMI overpass time of 13:30 local standard time for the NO_2 vertical column total (left) and NO_2 model surface model layer (right). The annotation in the lower left provides the mean (min, max) values within the study domain.

Model performance

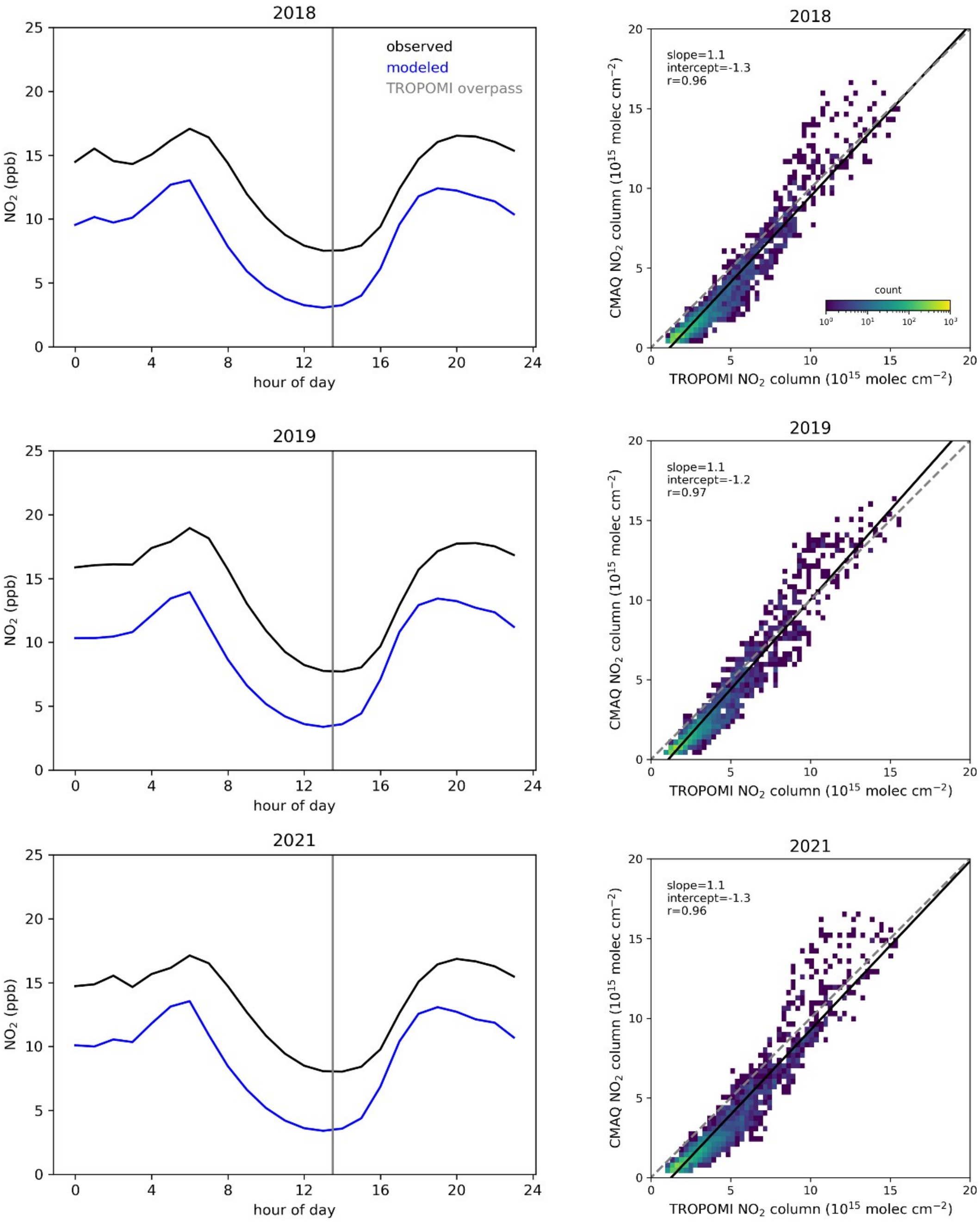

Figure S5. Performance of CMAQ-simulated NO_2 in September-November 2018, 2019, and 2021 compared to surface observations (left) and TROPOMI vertical column densities (right). For the surface monitoring sites, observed and modeled NO_2 are aggregated by hour across all sites in the CMAQ modeling domain. The TROPOMI overpass time of 13:30 local time is indicated with a grey vertical line. The comparison of vertical columns is for the average vertical column over the September-November study period. A one-to-one line is shown as a dashed grey line, and the linear regression between TROPOMI and CMAQ vertical columns is shown as a solid black line. The color scale represents the count of CMAQ/TROPOMI paired values that fall within each bin.

Table S2. Performance for NO_2, relative humidity (RH), temperature, and wind speed compared to surface monitoring sites. Statistics include mean bias (MB), normalized mean bias (NMB), and correlation coefficient (r).

		2018	2019	2021
NO_2	MB (ppb)	-4.5	-4.8	-4.4
	NMB (%)	-34	-34	-32
	r	0.63	0.65	0.68
RH	MB (%)	-6.9	-7.0	-8.6
	NMB (%)	-14	-16	-18
	r	0.86	0.86	0.86
Temperature	MB (°C)	1.4	1.6	1.5
	NMB (%)	7.1	8.2	7.7
	r	0.93	0.94	0.93
Wind speed	MB (m/s)	0.9	0.9	0.9
	NMB (%)	48	49	47
	r	0.62	0.63	0.61

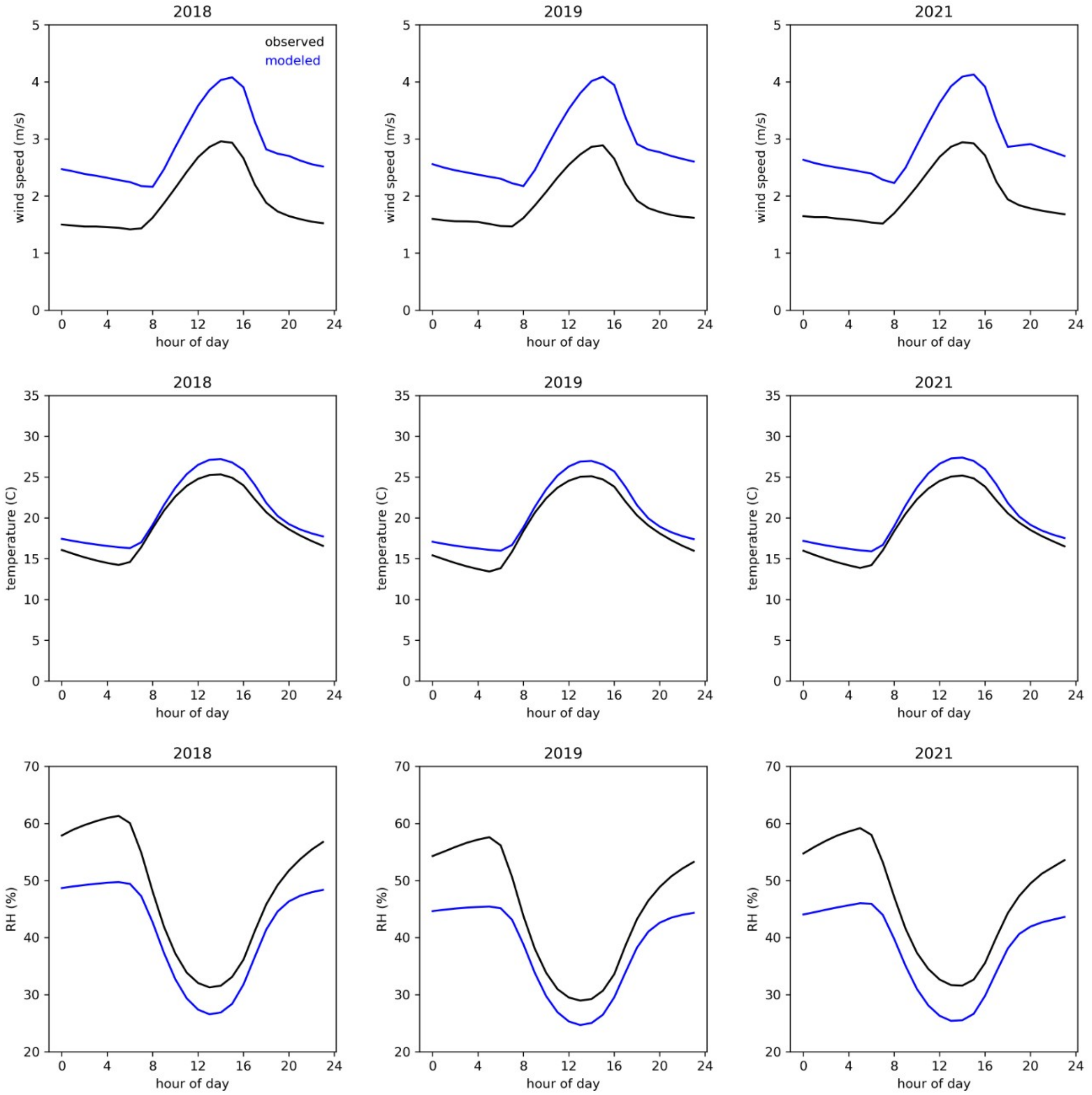

Figure S6. Performance of simulated meteorology in September-November 2018, 2019, and 2021 compared to surface observations. Observed and modeled values are aggregated by hour across all sites in the CMAQ modeling domain.

Wind direction analysis

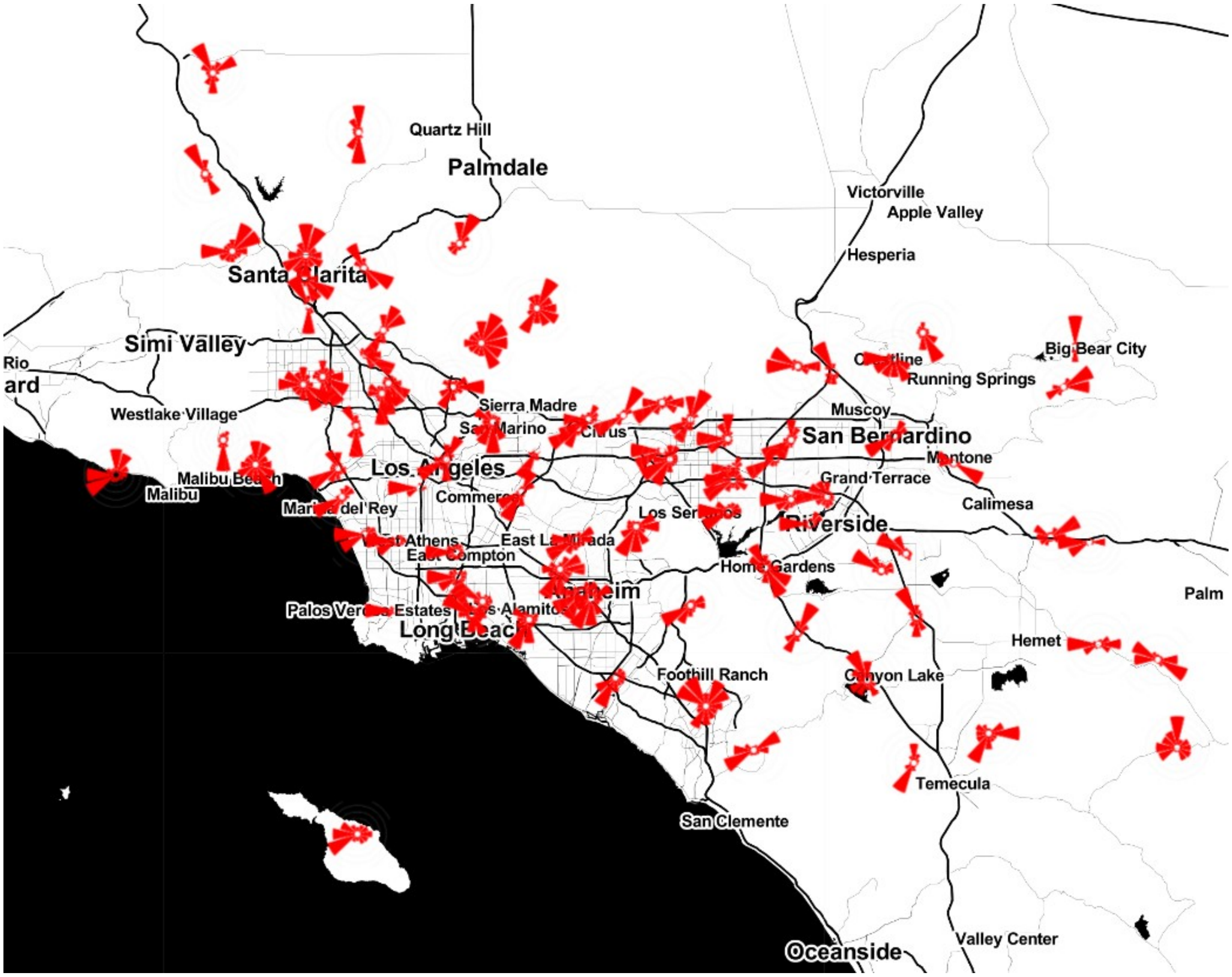

Figure S7. Wind roses of hourly data measured at meteorological stations in the Los Angeles basin during September-November 2021.

Statistical significance of changes in TROPOMI NO_2

To determine whether the changes in TROPOMI NO_2 are statistically significant, we compare the changes to the estimated error in TROPOMI NO_2 retrievals. According to the TROPOMI NO_2 product Algorithm Theoretical Basis Document (https://sentinel.esa.int/documents/247904/2476257/Sentinel-5P-TROPOMI-ATBD-NO2-data-products), the error for an individual tropospheric NO_2 retrieval is approximately 0.5×10^{15} molecules/cm^2 + [0.2 to 0.5]$\cdot N_v^{trop}$ where N_v^{trop} is the tropospheric NO_2 vertical column total. We take the midpoint of the 0.2 to 0.5 range and use 0.35 as the tropospheric column multiplier. The TROPOMI NO_2 columns are averaged over September-November as part of the oversampling process. We calculate the error in an individual day's column (ε_{daily}) using the error formula above. The average error (ε_{avg}) is then the error for one day divided by the square root of the number of days (n) which in our case is 91 days covering September 1 – November 30.

$$\varepsilon_{daily} = 0.5 + 0.35 \cdot N_v^{trop}\, molecules/cm^2$$

$$\varepsilon_{avg} = \frac{\varepsilon_{daily}}{\sqrt{n}}$$

A change in TROPOMI is considered statistically significant if its absolute value exceeds the sum of the error in the 2018-2019 September-November NO_2 column and the error in the 2021 September-November NO_2 column on a grid cell by grid cell basis. Figure S8 shows the changes in TROPOMI NO_2 (as in Figure 4 of the main text) with grid cells where the changes are not statistically significant filled with grey.

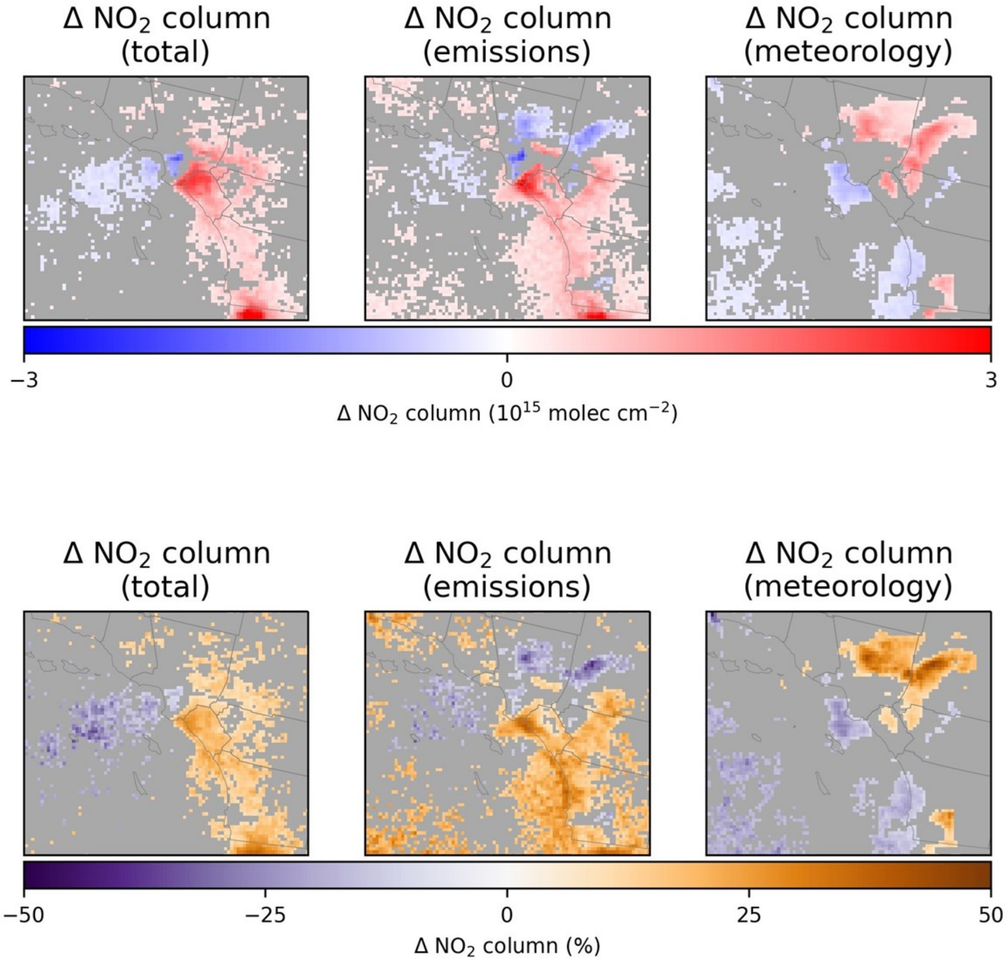

Figure S8. Total change (left) in TROPOMI NO_2 column in September-November 2021 compared to the average over the same period in 2018 and 2019. Total changes are apportioned to emissions (middle) and meteorology (right) using a meteorological adjustment derived from CMAQ simulations. Both absolute changes (top row) and percent changes (bottom row) are shown. Grid cells where the changes are not statistically significant are filled with grey.

Change in surface NO_2 compared to change in TROPOMI NO_2

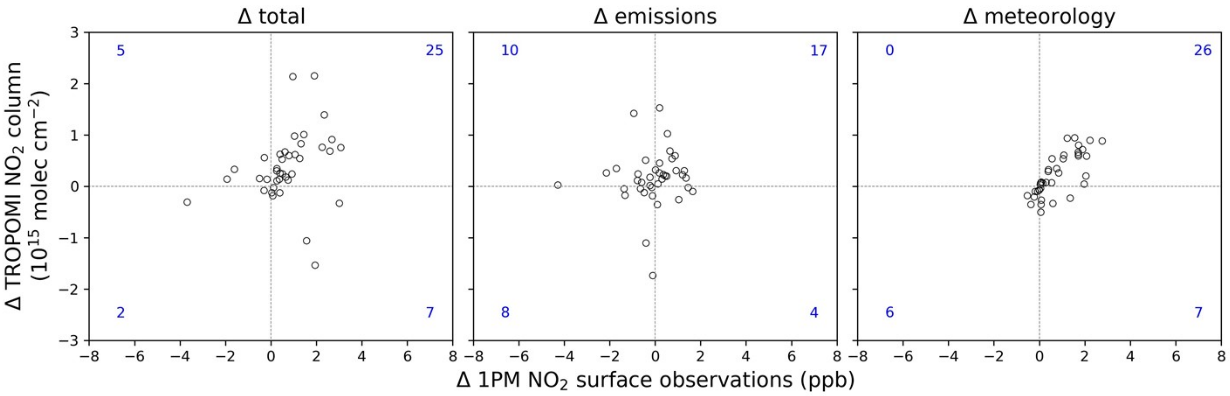

Figure S9. Change in 1-2 pm surface NO_2 compared to change in TROPOMI NO_2 column. Values are the average in September-November 2021 compared to the average values in September-November 2018 and 2019. The number in the corner of each quadrant shows the count of data pairings falling within that quadrant. Data in the upper right and lower left quadrants are points where the change in surface NO_2 and TROPOMI NO_2 agree in direction.

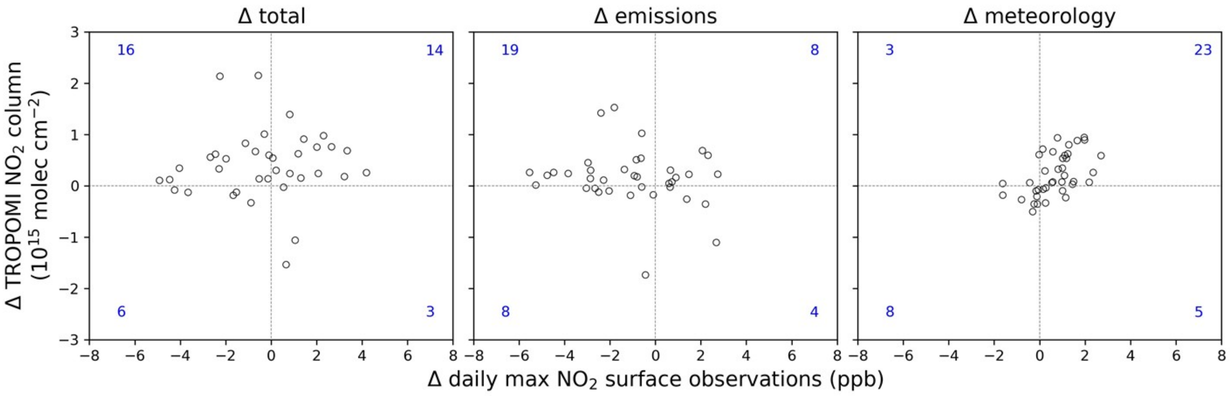

Figure S10. Change in daily max surface NO_2 compared to change in TROPOMI NO_2 column. Values are the average in September-November 2021 compared to the average values in September-November 2018 and 2019. The number in the corner of each quadrant shows the count of data pairings falling within that quadrant. Data in the upper right and lower left quadrants are points where the change in surface NO_2 and TROPOMI NO_2 agree in direction.

CMAQ meteorological adjustment to $PM_{2.5}$

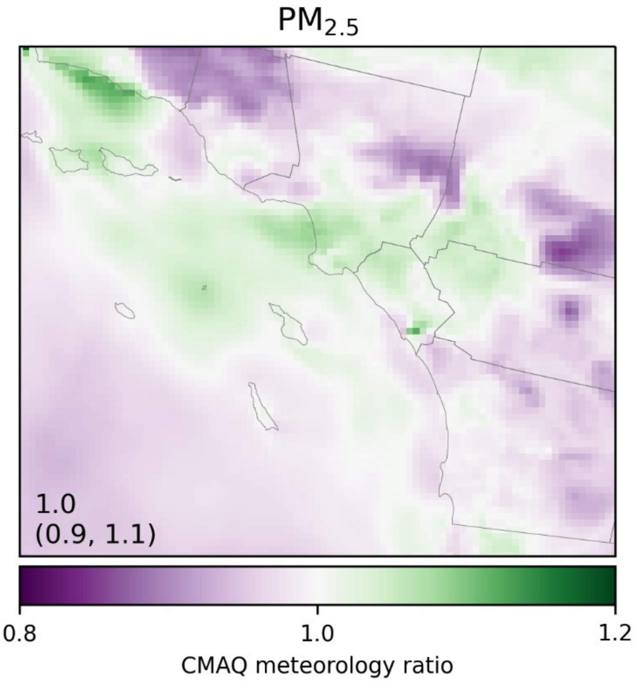

Figure S11. The CMAQ meteorology ratio described in Eq. 1 of the main text. The results shown here are for the average of September-November for 2018 and 2019 for daily average $PM_{2.5}$ concentration. The annotation in the lower left provides the mean (min, max) values within the study domain.

PM$_{2.5}$ species concentrations

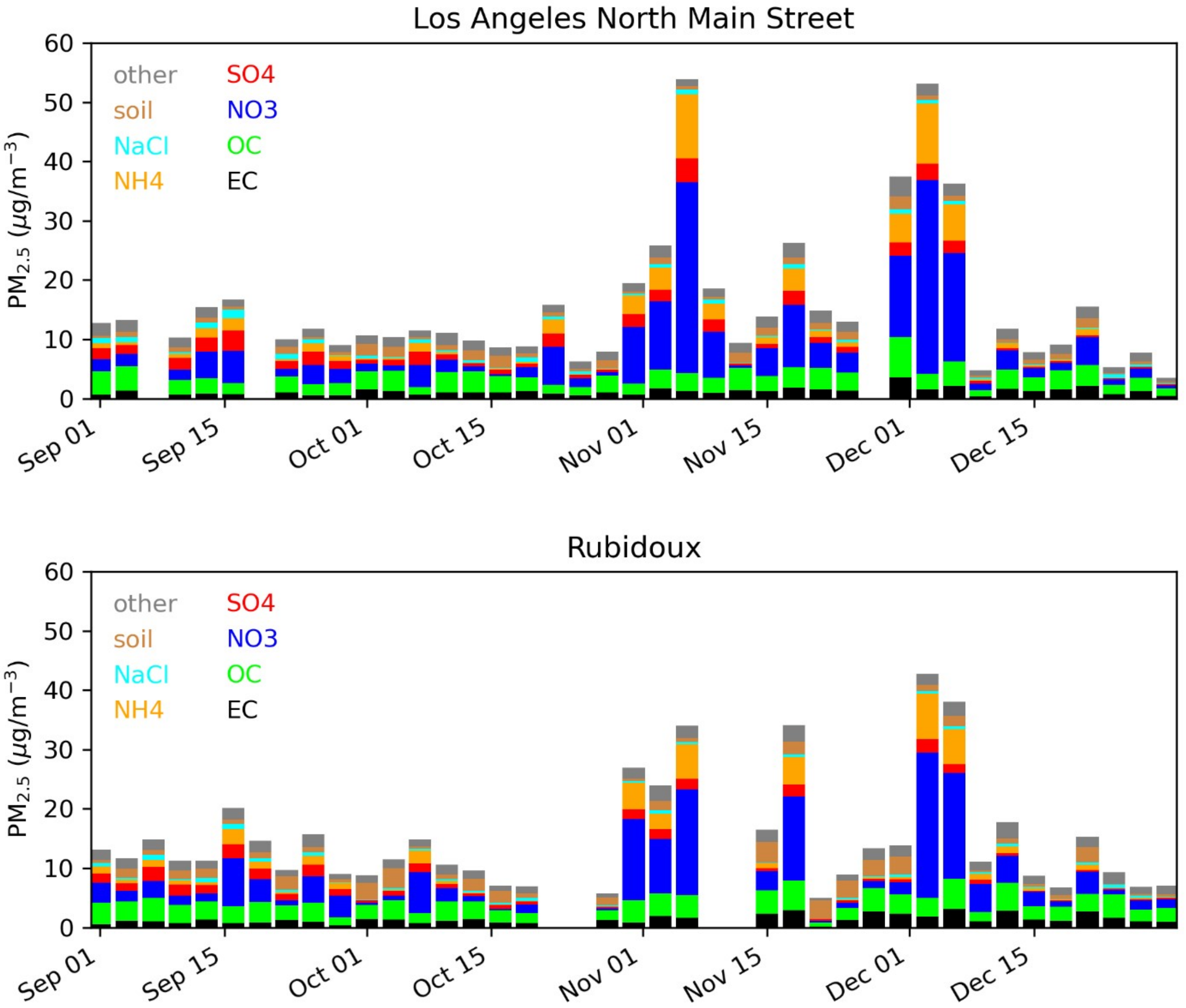

Figure S12. PM$_{2.5}$ species concentrations measured at the Los Angeles North Main Street and Rubidoux Chemical Speciation Network (CSN) sites during September – December 2021. Days that have missing data for some species have been excluded. EC = elemental carbon; OC = organic carbon; NO3 = nitrate; SO4 = sulfate; NH4 = ammonium; NaCl = sodium chloride (i.e., sea salt). Figure S13 shows the locations of these sites within the study domain.

Figure S13. Locations of Los Angeles North Main Street and Rubidoux CSN sites referenced in Figure S12.

Changes in TROPOMI column totals compared to major roadway locations

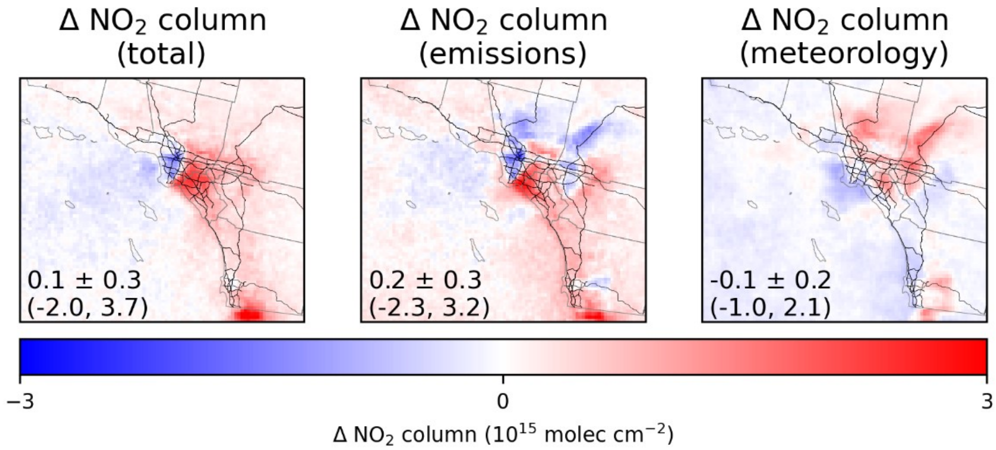

Figure S14. Total change in TROPOMI NO_2 column in September-November 2021 compared to the average over the same period in 2018 and 2019 (left). Total changes are apportioned to emissions (middle) and meteorology (right) using a meteorological adjustment derived from CMAQ simulations. The annotations in the lower left of each panel show the mean ± standard deviation (min, max) over land grid cells.

Caltrans Performance Monitoring System VMT data

In addition to the changes in total vehicle flow, we also examined the changes in total VMT and truck VMT in five counties making up most of the study domain (Figure S15; Table S3). Total VMT was reduced in September – November 2021 compared to the baseline during the same period in 2018-2019. The largest reductions in total VMT occurred in San Bernardino County while Riverside and Ventura counties also saw large reductions. Total VMT also decreased in Los Angeles and Orange Counties by smaller amounts. Changes in truck VMT sometimes differed from the changes in total VMT. This is most notable in San Bernardino County. Despite having the largest reduction in total VMT of the five counties examined here, San Bernardino County experienced the largest increase in truck VMT. Orange County also saw an increase in truck VMT despite decreases in total VMT. The correspondence of changes in VMT with changes in NO_2 and $PM_{2.5}$ is mixed. There is decreased VMT (total and truck) in Los Angeles County, which is consistent with a decrease in emission influenced NO_2 throughout most of the county; however, the emission influenced $PM_{2.5}$ increased in Los Angeles County increased at most sites. In Orange County where the largest increases in emission influenced column NO_2 were found, there was a decrease in total VMT and an increase in truck VMT. The effects of emissions on NO_2 in San Bernardino County were mixed, with some areas increasing and others decreasing, but $PM_{2.5}$ almost universally increased. There was a large increase in truck VMT in San Bernardino County during this time. In both Ventura and Riverside Counties, emission influenced column NO_2 mostly increased with some smaller areas showing decreases while total and truck VMT decreased in both counties. $PM_{2.5}$ decreased at sites in Ventura County while $PM_{2.5}$ increased at most sites in Riverside County. Overall, we do not find any consistent relationships between the changes in VMT and the changes in NO_2 or $PM_{2.5}$ in these counties.

Table S3. Change in total VMT and truck VMT during September-November 2021 compared to the average over the same period in 2018 and 2019 for five counties near the Los Angeles metropolitan area.

County	2021 VMT change	2021 truck VMT change
Los Angeles	-4.0%	-7.7%
Orange	-4.4%	5.3%
San Bernardino	-16.9%	15.9%
Riverside	-14.1%	-8.8%
Ventura	-14.4%	-19.8%

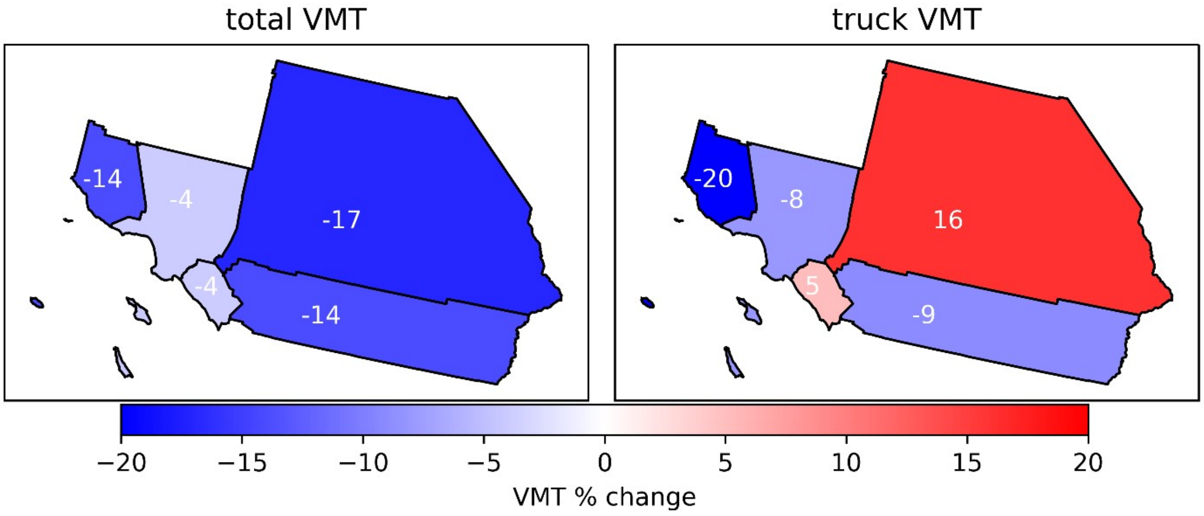

Figure S15. Percent change in total VMT and truck VMT by county during September – November 2021 compared to the average during the same period in 2018 and 2019.