TROPOMI NO2 in the United States: A detailed look at the annual averages, weekly cycles, effects of temperature, and correlation with PM2.5

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Abstract

Observing the spatial heterogeneities of NO2 air pollution is an important first step in quantifying NOx emissions and exposures. This study investigates the capabilities of the Tropospheric Monitoring Instrument (TROPOMI) in observing the spatial and temporal patterns of NO2 pollution in the Continental United States (CONUS). The high instrument sensitivity can differentiate the fine-scale spatial heterogeneities in urban areas, such as hotspots related to airport/shipping operations and high traffic areas, and the relatively small emission sources in rural areas, such as power plants and mining operations. We also examine NO2 columns by day-of-the-week and find that Saturday and Sunday concentrations are 16% and 24% lower respectively than during weekdays. In cities with topographic features that inhibit dispersion, such as Los Angeles, there appears to be a pollution build-up from Monday through Friday, while cities which have better dispersion have more variability during weekdays. We also analyze the correlation of temperatures and NO2 column amounts and find that NO2 is larger on the hottest days (>32C) as compared to warm days (26C - 32C), which is in contrast to a general decrease in NO2 with increasing temperature at lower temperature bins. Finally, we compare column NO2 with estimates of surface PM2.5 and find fairly poor correlation, suggesting that NO2 and PM2.5 are becoming increasingly less correlated in CONUS. These new developments make TROPOMI NO2 satellite data advantageous for policymakers and public health officials, who request information at high spatial resolution and short timescales, in order to assess, devise, and evaluate regulations.

TROPOMI NO_2 in the United States: A detailed look at the annual averages, weekly cycles, effects of temperature, and correlation with $PM_{2.5}$

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Abstract

Observing the spatial heterogeneities of NO_2 air pollution is an important first step in quantifying NO_X emissions and exposures. This study investigates the capabilities of the Tropospheric Monitoring Instrument (TROPOMI) in observing the spatial and temporal patterns of NO_2 pollution in the Continental United States (CONUS). The high instrument sensitivity can differentiate the fine-scale spatial heterogeneities in urban areas, such as hotspots related to airport/shipping operations and high traffic areas, and the relatively small emission sources in rural areas, such as power plants and mining operations. We also examine NO_2 columns by day-of-the-week and find that Saturday and Sunday concentrations are 16% and 24% lower respectively than during weekdays. In cities with topographic features that inhibit dispersion, such as Los Angeles, there appears to be a pollution build-up from Monday through Friday, while cities which have better dispersion have more variability during weekdays. We also analyze the correlation of temperatures and NO_2 column amounts and find that NO_2 is larger on the hottest days (>32°C) as compared to warm days (26°C - 32°C), which is in contrast to a general decrease in NO_2 with increasing temperature at lower temperature bins. Finally, we compare column NO_2 with estimates of surface $PM_{2.5}$ and find fairly poor correlation, suggesting that NO_2 and $PM_{2.5}$ are becoming increasingly less correlated in CONUS. These new developments make TROPOMI NO_2 satellite data advantageous for policymakers and public health officials, who request information at high spatial resolution and short timescales, in order to assess, devise, and evaluate regulations.

Introduction

Enhancements of NO_2 serve as a stark reminder of our society's global reliance on fossil-fuel combustion. NO_2 – which comprises ~70% of NO_X ($NO_X = NO + NO_2$) in urban airsheds (Valin et al., 2013) – primarily originates as a byproduct of fossil-fuel combustion, although there are some biogenic sources of NO_2 such as lightning and microbes in soil (Jacob, 2000). NO_2 is a toxic air pollutant, which can cause and exacerbate asthma in vulnerable populations (Achakulwisut et al., 2019; Anenberg et al., 2018) and lead to premature mortality (Burnett et al., 2004). NO_2 can also react in the atmosphere to create tropospheric ozone (O_3), which is noted for its damaging effects including premature aging of lungs (Broeckaert et al., 1999; McConnell et al., 2002) and premature mortality (Bell, 2004; Bell et al., 2006). HNO_3 often represents the final chemical state of NO_2 in the atmosphere and when deposited, agitates the equilibrium of our ecosystems due to its acidic properties (Burns et al., 2016). NO_2 can also participate in a series of reactions to create particulate nitrate (NO_3^-), a component of fine particulate matter less than 2.5 microns in diameter ($PM_{2.5}$), which is the leading cause of mortality due to air pollution (Cohen et al., 2017).

There is a rich legacy of monitoring NO_2 by remote sensing instruments (Burrows et al., 1999). NO_2 can be observed from space because it has unique high-frequency spectral features within the 400 – 500 nm wavelength region (Vandaele et al., 1998). The newest remote sensing spectrometer, TROPOMI (VanGeffen et al., 2019; Veefkind et al., 2012), has been gathering data on the global heterogeneities of NO_2 air pollution since October 2017. This instrument builds on the legacy of prior Ultraviolet – Visible (UV-Vis) spectrometers including the Global Ozone Monitoring Experiment (GOME) (Burrows et al., 1999; Martin et al., 2002; Richter & Burrows, 2002), the Scanning Imaging Spectrometer for Atmospheric Chartography (SCIAMACHY) (Bovensmann et al., 1999; Heue et al., 2005), the Global Ozone Monitoring Experiment - 2 (GOME-2) instrument (Munro et al., 2016; Richter et al., 2011), and the Ozone Monitoring Instrument (OMI) (Boersma et al., 2018; Krotkov et al., 2017; Levelt et al., 2006, 2018).

Satellite-based remote sensing instruments can be particularly useful in quantifying the trends of NO_X pollution in high-emission areas (Castellanos & Boersma, 2012; Duncan et al., 2016; Georgoulias et al., 2019; Krotkov et al., 2016; McLinden et al., 2016; Stavrakou et al., 2008; Van

Der A et al., 2008), the seasonal cycles of air pollution (Ialongo et al., 2016; Shah et al., 2020), and the weekly cycle of NO_X emissions (Beirle et al., 2003; Ialongo et al., 2016; Ma et al., 2013; Russell et al., 2010; Valin et al., 2014). In an additional step, NO_X emissions can be computed by combining the satellite data with meteorological information (Beirle et al., 2011, 2019; de Foy et al., 2015; Goldberg, Lu, Streets, et al., 2019; Goldberg, Saide, et al., 2019; Lorente et al., 2019; Lu et al., 2015; Valin et al., 2013) or by combining the satellite data with chemical transport models (Canty et al., 2015; Cooper et al., 2017; Qu et al., 2017; Souri et al., 2016). Due to the consistency and robustness of the remotely-sensed NO_2 data record, scientists are beginning to infer information from the NO_2 data about other trace gases such as CO_2 (Goldberg, Lu, Oda, et al., 2019; Konovalov et al., 2016; Reuter et al., 2019), CH_4 (de Gouw et al., 2020), and CO (Lama et al., n.d.), since remotely-sensed measurements of those trace gases are generally less reliable. Therefore, remotely-sensed NO_2 can also be helpful in indirectly estimating greenhouse gas emissions.

TROPOMI's smallest pixel size (3.5×7.2 km^2 at nadir, reduced to 3.5×5.6 km^2 at nadir on August 6, 2019) and enhanced sensitivity are significant improvements when compared to previous satellite instruments (Veefkind et al., 2012). NO_2 is unique due to its relatively short photochemical lifetime which varies from 2-5 h during the summer daytime (Beirle et al., 2011; de Foy et al., 2014; Laughner & Cohen, 2019; Valin et al., 2013) to 12-24 h during winter (Shah et al., 2020). As a result, tropospheric NO_2 concentrations are strongly correlated with local NO_X emissions, which are often anthropogenic in origin.

Initial NO_2 measurements from TROPOMI show the complex spatial heterogeneities of NO_2 pollution with more refined resolution than any instrument before it (Griffin et al., 2019; Ialongo et al., 2020). In particular, the smaller pixel sizes aid researchers in differentiating pollution sources within a single metropolitan area such as isolating signals from airports and individual highways (Judd et al., 2019). These small-scale pixel sizes also show better agreement with the spatial features suggested by ground-based measurements (Ialongo et al., 2020; Judd et al., 2019). In particular, modeling studies have shown that matching the NO_2 column to 10% accuracy requires a spatial resolution of at least 4 km (Valin et al., 2011) – the approximate spatial resolution of TROPOMI. Robust high-spatial resolution estimates are also critical inputs to those trying to quantify the surface-level NO_2 exposures (Geddes et al., 2016; Lamsal et al., 2008; Larkin et al., 2017).

The improved spatial resolution and instrument sensitivity also allows for shorter temporal averaging ranges (days to months) to gain the similar spatial structure it would normally take >1 year to gather (Beirle et al., 2019; Dix et al., 2020; Goldberg, Lu, Streets, et al., 2019; Lorente et al., 2019). As a result, it is easier to gain insight on the short-term variations of NO_X pollution when using TROPOMI, which can be especially helpful for those trying to quantify intra-annual changes in NO_X emissions (F. Liu et al., 2020).

In this paper, we exploit TROPOMI's small pixel sizes and enhanced instrument sensitivity to analyze spatial and temporal features of NO_X columns in the continental United States on annual, seasonal, weekly, and daily timescales. For example, using only a short temporal range of data, we can now answer such questions as:

- Which location within each U.S. state has the worst NO_2 air pollution?
- How does the NO_X emissions cycle vary by day of the week?
- How does temperature affect column NO_2 amounts?
- What is the relative magnitude of NO_2 compared to $PM_{2.5}$?

While older sensors (e.g., OMI) provided insight into some of these questions, early sensors lacked the same sensitivity and required longer oversampling times. Therefore, answers illuminated by TROPOMI provide a "clarity" that has not been seen before.

Methods

TROPOMI NO_2

TROPOMI was launched by the European Space Agency (ESA) for the European Union's Copernicus Sentinel 5 Precursor (S5p) satellite mission on October 13, 2017. The satellite follows a sun-synchronous, low-earth (825 km) orbit with an equator overpass time of approximately 13:30 local solar time (Veefkind et al., 2012). TROPOMI measures total column amounts of several trace gases in the Ultraviolet-Visible-Near Infrared-Shortwave Infrared spectral regions (VanGeffen et al., 2019). This instrument is characterized as a passive optical satellite sensor due to its reliance on solar UV-Visible radiation to gather measurements. At nadir, pixel sizes are 3.5 × 7 km^2 (reduced to 3.5 × 5.6 km^2 on August 6, 2019) with little variation in pixel sizes across the 2600 km swath. The instrument observes the swath approximately once every second and orbits the Earth in about 100 minutes, resulting in daily global coverage.

Using a differential optical absorption spectroscopy (DOAS) technique on the radiance measurements in the 405 – 465 nm spectral window, the top-of-atmosphere spectral radiances can be converted into slant column amounts of NO_2 between the sensor and the Earth's surface (van Geffen et al., 2020). In two additional steps, the slant column quantity can be converted into a tropospheric vertical column content. In the first step, the stratospheric portion of the column (the amount above approximately 12 km in altitude) is subtracted either by using a measurement in a remote area or by using a global model estimate. In a second step, the slant tropospheric column is converted to a vertical column using a quantity known as the air mass factor. The air mass factor is the most uncertain quantity in the retrieval algorithm (Lorente et al., 2017), and is a function of the surface reflectance, the NO_2 vertical profile, and scattering in the atmosphere among other factors. Using accurate and high-resolution data (spatially and temporally) as inputs in calculating the air mass factor can significantly reduce the overall errors of the air mass factor (S. Choi et al., 2019; Goldberg et al., 2017; Laughner et al., 2016, 2019; Lin et al., 2015; M. Liu et al., 2019; Russell et al., 2011; Zhao et al., 2020) and thus the tropospheric vertical column content.

Operationally, the TM5-MP model (1 × 1° resolution) is used to provide the NO_2 vertical shape profile and the climatological Lambertian Equivalent Reflectivity (0.5 × 0.5° resolution) (Kleipool et al., 2008) is used to provide the surface reflectivities. The operational air mass factor calculation does not explicitly account for aerosol absorption effects, which are accounted for in the effective cloud radiance fraction. While the operational product does have larger uncertainties in the tropospheric column contents than a product with higher spatial resolution inputs, we limit our analysis to relative trends, which dramatically reduces this uncertainty.

Re-gridding

For our analysis we re-grid the operational TROPOMI tropospheric vertical column NO_2, with native pixels of approximately 3.5 × 7 km^2, to a newly defined 0.01° × 0.01° grid (approximately 1 × 1 km^2) centered over the continental United States (CONUS; corner points: SW: 24.5° N, 124.75° W; NE: 49.5° N, 66.75° W). Before re-gridding, the data are filtered so as to use only the highest quality measurements (quality assurance flag (QA_flag) > 0.75). Once the re-gridding has been completed, the data is averaged over varying timeframes as discussed in the results section.

Other Datasets

Additionally, we use two complementary products in some sections of our analysis. When filtering the data based on temperature, we use the maximum daily hourly 2-meter temperature (T2m-Max) from the ERA5 re-analysis. To downscale the ERA5 re-analysis, which is provided at 0.25° × 0.25°, we spatially interpolate daily T2m-Max to 0.01° × 0.01° using bilinear interpolation. For that reason, the heat-urban island effect and any microscale meteorology features (e.g., sea breezes) will not be accounted for, but these effects should be minor for our particular analysis, which groups temperatures in 5° C intervals. We also compare our 0.01° × 0.01° TROPOMI NO_2 data to an annual $PM_{2.5}$ dataset at the same spatial resolution (VanDonkelaar et al., 2019).

Results

TROPOMI NO_2 in CONUS

Figure 1 depicts the 2019 CONUS annual average of TROPOMI tropospheric vertical column NO_2 compared to averages over shorter timeframes.

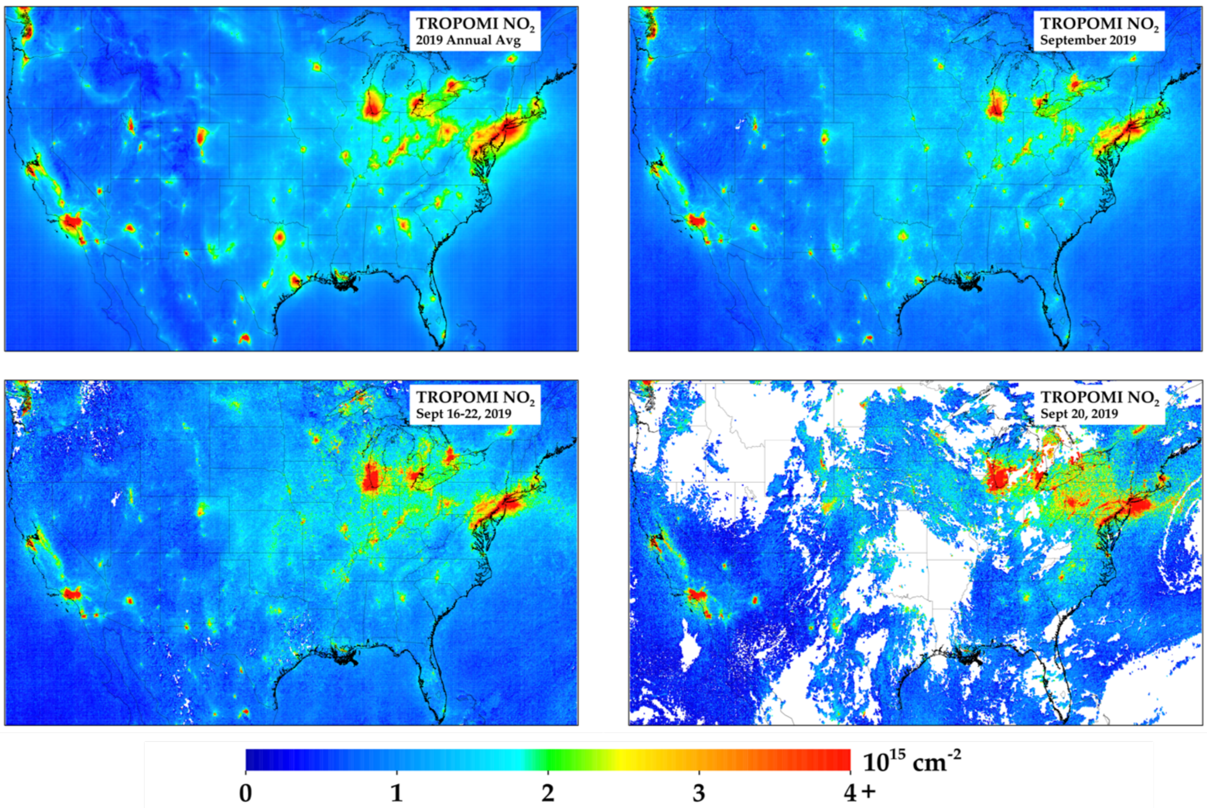

Figure 1. TROPOMI NO_2 oversampled to 0.01° × 0.01° spatial resolution for four different temporal resolutions: (top left) annual, (top right) monthly, (bottom left) weekly, and (bottom right) daily.

This example illustrates how shorter timeframes compare to the annual average in both magnitude and clarity. In the single daily snapshot (September 20, 2019), there are wide sections that are missing due to cloud coverage. In the areas that do have coverage, values can be a factor of five different than the annual average, but the spatial heterogeneities are generally captured. When oversampling over a one-week period (September 16 – 22, 2019), the image quickly starts to resemble the annual average with some differences in magnitude due to meteorological factors, such as temperature (which will be discussed later). The one-week average can therefore be considered the minimum amount of oversampling time to properly capture spatial heterogeneities. A monthly oversampled image essentially captures the same spatial heterogeneities as the annual average, but with magnitude differences due to meteorology. It should be noted that September was specifically chosen for this analysis due to its propensity to have both less cloud coverage and snow cover than other months. If oversampling during winter months (i.e., Dec – March), which tend to have fewer ideal conditions for satellite retrievals of trace gases, oversampling times will need to be longer to achieve similar clarity.

When visually inspecting the CONUS TROPOMI NO_2 average during the initial twenty months of the TROPOMI record (May 1, 2018 – Dec 31, 2019) (Figure 2), we now start to see clear spatial heterogeneities across the domain. The largest U.S. cities can be seen and their magnitudes can be compared to each other (results further discussed later).

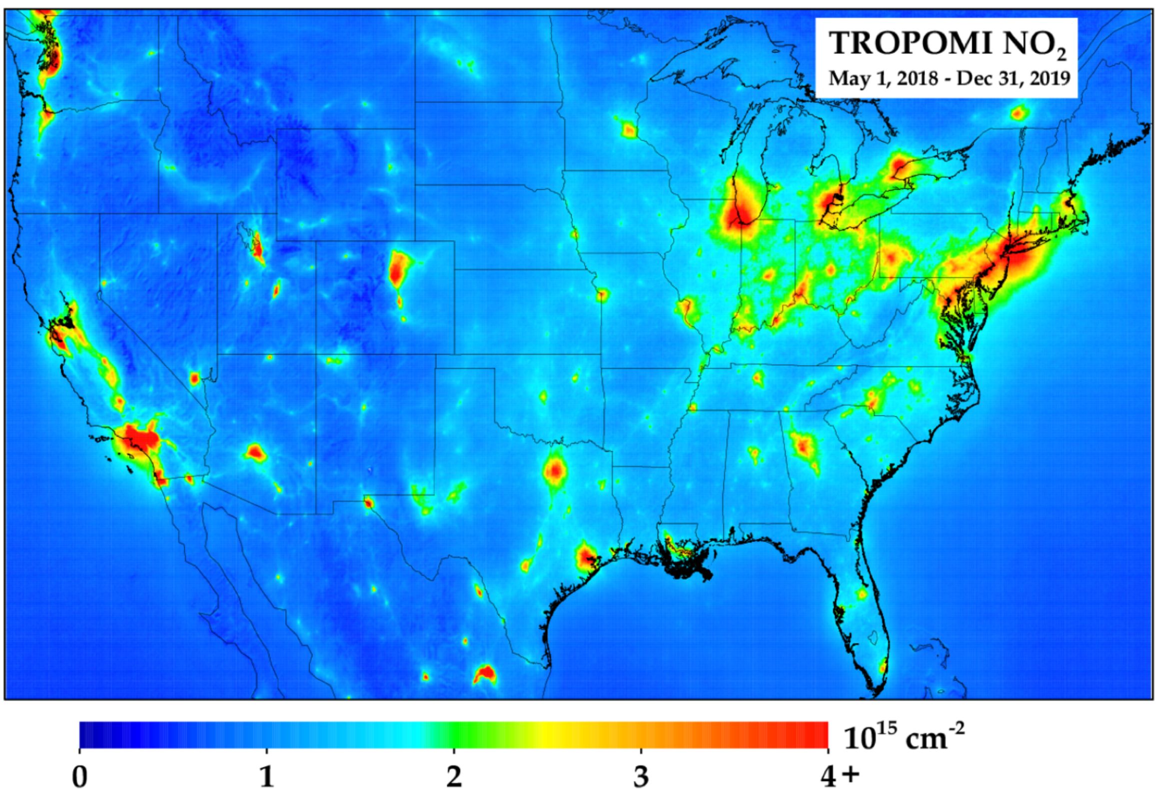

Figure 2. TROPOMI NO_2 oversampled to 0.01° × 0.01° spatial resolution during May 1, 2018 – December 31, 2019. Only pixels exceeding a quality assurance flag of 0.75 are included.

Equally important, smaller sources of NO_2 pollution can now be observed, and they are not spatially smeared into the background NO_2 concentration. For example, when magnifying the western United States (Figure 3), the roadway network and related activity in the Idaho Snake River valley can be clearly observed. Other examples are the copper mining operations in eastern Arizona associated with the Morenci Mine, the coal mining operations in the Powder River Basin in eastern Wyoming, and to a lesser extent the gold mining operations associated with the Goldstrike mine in Nevada. In addition, NO_2 concentrations are clearly correlated with oil & gas operations in the Permian (Texas) and Bakken (North Dakota) basins (also discussed in (Dix et al., 2020)) and is > 5 times larger than the NO_2 in the rural areas upwind. Individual spikes in NO_2 associated with NO_X emissions from large power plants (e.g., Navajo in Arizona, Craig in Colorado, Colstrip in Montana, North Valmy in Nevada, Four Corners/San Juan in New Mexico, Intermountain, Bonanza, Hunter/Huntington in Utah, Jim Bridger in Wyoming) can also be observed during this 2018-2019 period even though there have been large reductions (~85%) in the NO_X emissions from most of these power plants since the introduction of the federally-mandated NO_X SIP call in 2003.

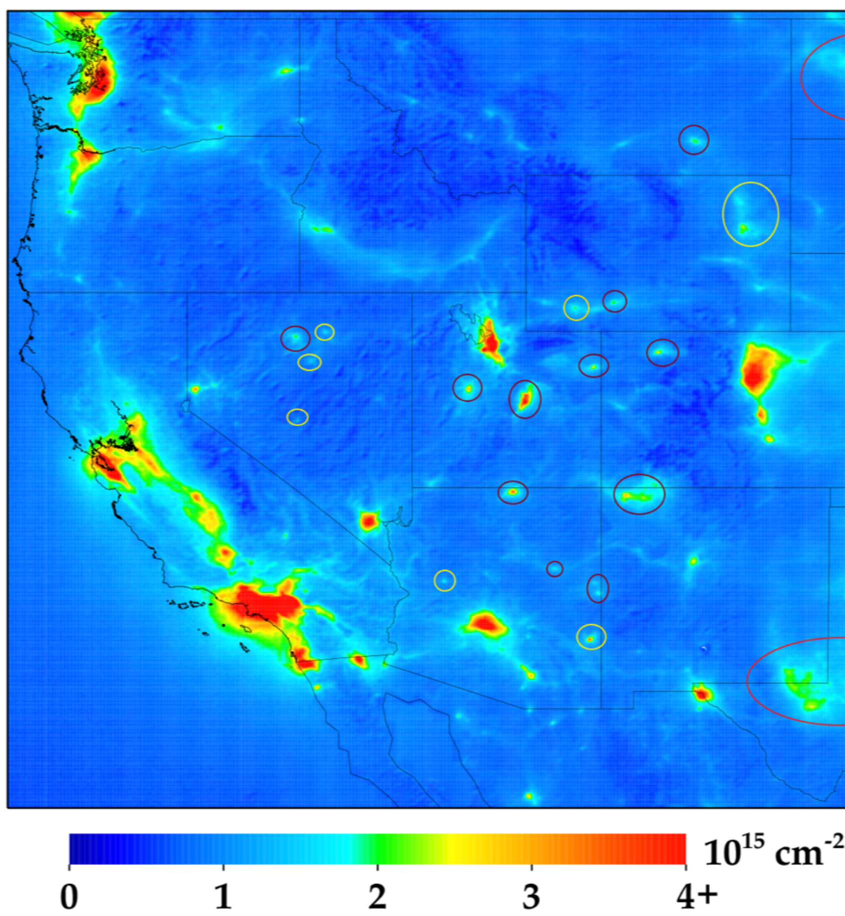

Figure 3. Same data shown in Figure 2, but now zoomed into the western United States. Power plants are outlined in dark magenta, mining operations in yellow, and oil & gas in bright red.

TROPOMI data is especially powerful in analyzing local variations in NO_2 pollution as compared to predecessor instruments. In Figure 4, we zoom into five different U.S. states, and in Table 1 we provide the largest NO_2 values in each state.

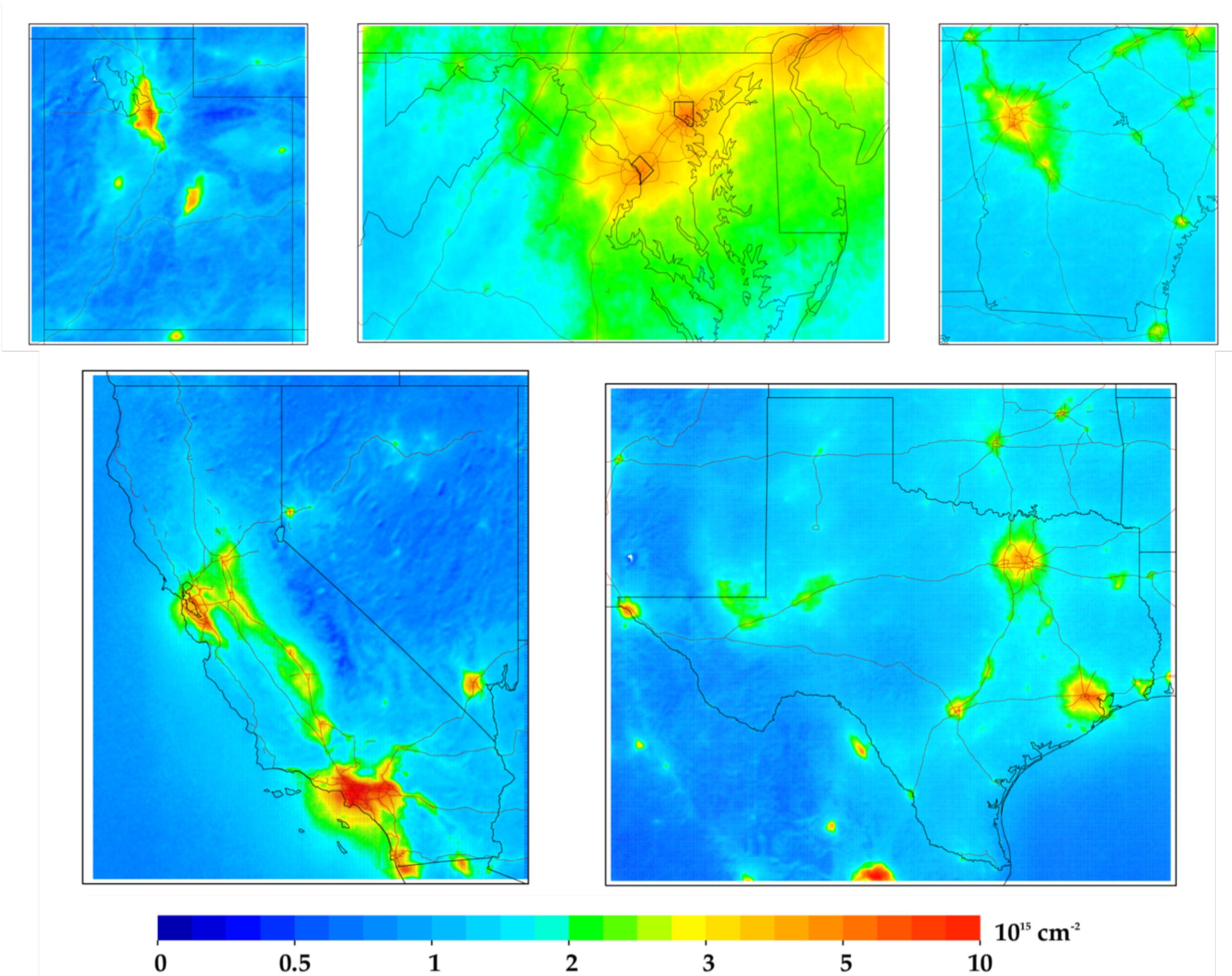

Figure 4. Same data shown in Figure 2, but now zoomed into 5 different U.S. states. Color bar has been adjusted to better differentiate spatial heterogeneities on a local scale.

Table 1. Largest NO_2 column value in each U.S. state during the May 1, 2018 – Dec 31, 2018 period. Ordered by largest to smallest maximum value.

State	Lat	Lon	Value	Detailed location
CA	34.03	-118.18	1.41E+16	E Los Angeles, CA
NY	40.72	-73.97	1.13E+16	East River, Brooklyn, NY
NJ	40.69	-74.14	9.75E+15	Port Newark, NJ
IL	41.82	-87.77	7.31E+15	Cicero, Chicago, IL (near MDW)
WA	47.46	-122.26	6.90E+15	Tukwila, WA (SE Seatle)
IN	41.66	-87.47	6.28E+15	E Chicago, IN (Steel Mill)
UT	40.71	-111.9	6.18E+15	S Salt Lake City, UT
CO	39.76	-105.02	5.98E+15	Highland, Denver, CO
PA	39.95	-75.16	5.95E+15	Downtown Philadelphia, PA
AZ	33.47	-112.15	5.87E+15	Cuatro Palmas, Phoenix, AZ
MI	42.31	-83.11	5.74E+15	Detroit, MI
TX	29.74	-95.14	5.58E+15	Deer Park, Houston, TX
CT	41	-73.67	5.46E+15	Greenwich, CT
NV	36.1	-115.18	4.97E+15	Las Vegas Strip, Las Vegas, NV
MD	39.28	-76.6	4.94E+15	Port of Baltimore, Baltimore, MD
DC	38.89	-77.01	4.65E+15	Capitol Hill, Washington, DC
GA	33.64	-84.42	4.65E+15	Hartsfield Airport, Atlanta, GA
VA	38.88	-77.05	4.59E+15	Pentagon, Arlington, VA
DE	39.8	-75.37	4.34E+15	Claymont, Wilmington, DE
OR	45.52	-122.65	4.25E+15	Buckman, Portland, OR
KY	38.18	-85.73	4.21E+15	Louisville, KY (Airport)
OH	39.12	-84.54	4.20E+15	Cincinatti, OH
MA	42.37	-71.06	4.14E+15	Charlestown, Boston, MA (near BOS)
LA	29.93	-90.14	3.98E+15	Mississippi River, New Orleans, LA
NC	35.24	-80.85	3.76E+15	Catawba, NC (near Marshall Steam SPP)
WV	38.94	-82.11	3.68E+15	Lakin, WV (near Gavin PP)
MO	38.68	-90.19	3.67E+15	Mississippi River, St Louis, MO
KS	39.12	-94.6	3.61E+15	Missouri River, Kansas City, KS
TN	36.16	-86.77	3.52E+15	Nashville, TN
FL	25.85	-80.34	3.40E+15	Medley, Miami, FL
WI	42.86	-87.82	3.40E+15	Oak Creek, WI (near Oak Creek PP)
MN	44.97	-93.24	3.28E+15	Mississippi River, Minneapolis, MN
AL	33.52	-86.82	3.21E+15	Fountain Heights, Birmingham, AL
RI	41.8	-71.41	2.88E+15	S Providence, RI
IA	41.25	-95.88	2.79E+15	Council Bluffs, IA
NE	41.25	-95.88	2.79E+15	Missouri River, Omaha, NE
OK	36.16	-96	2.64E+15	Tulsa, OK
WY	43.69	-105.32	2.52E+15	Thunder Basin Coal, WY
SC	32.88	-79.99	2.52E+15	N Charleston, SC
NM	35.11	-106.62	2.51E+15	Albuquerque, NM
AR	35.12	-90.1	2.46E+15	W Memphis, AR
ID	43.58	-116.23	2.30E+15	Boise, ID (Airport)
ND	47.35	-101.81	2.24E+15	Beulah, ND (near Dakota Gasification Co)
MT	45.86	-106.57	2.20E+15	Colstrip, MT (near Colstrip PP)
NH	42.94	-70.81	1.93E+15	Hampton, NH
ME	43.66	-70.29	1.90E+15	Portland, ME
MS	32.34	-90.19	1.77E+15	Jackson, MS
SD	43.6	-96.74	1.53E+15	N Sioux Falls, SD
VT	42.91	-73.18	1.49E+15	Wilmington, VT

In Figure 5, we zoom into six different U.S. cities. In each instance, the oversampled TROPOMI NO_2 images exhibit features that match known NO_X emissions patterns. The larger NO_2 values correlate very well to the interstate network, population density, and industrial activity hubs (such as manufacturing facilities, airports, and shipping ports). For example, in the image of Maryland, the largest value is observed at the Baltimore Harbor, which is a confluence of several major highways, a large shipping port, the city incinerator, and many industrial facilities. Similarly, the largest values in Chicago exist along the I-55 corridor which has a high traffic volume and a high-density of industrial facilities, with secondary maxima at the O'Hare International airport and the U.S. Steel mill in East Chicago, Indiana. In Los Angeles, the spatial pattern matches the basin outline very well, with the largest values between downtown Los Angeles and Long Beach. In Houston, Texas the largest values are nearest to the petrochemical refining facilities east of town. For all cases, TROPOMI can accurately quantify the relative relationship between the largest sources of NO_X emissions and NO_2 concentrations.

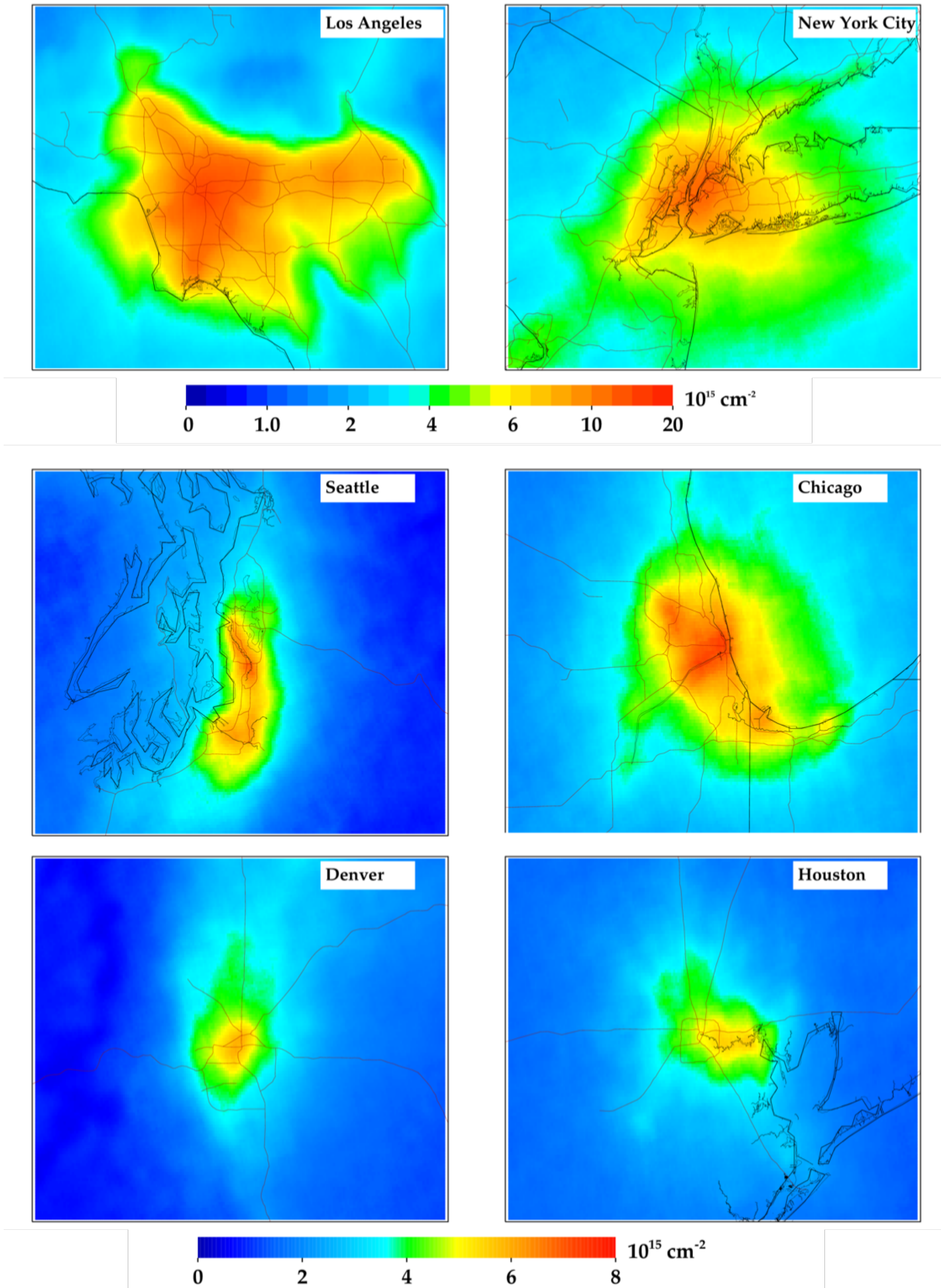

Figure 5. Same data shown in Figure 2, but now zoomed into 6 different U.S. cities. Color bar has been adjusted to better differentiate spatial heterogeneities on a local scale.

Day-of-the-week relationships

A common use of oversampled satellite data is in investigating the weekly cycle of NO_X emissions. In Figure 6, we show the weekly pattern of NO_2 across CONUS for three different days of the week as well as the full weekly cycle in seven U.S. cities. In all cities, the NO_2 appears to be approximately equivalent amongst all weekdays with some minor exceptions. NO_2 pollution is 2.5% larger on Tuesday than a typical weekday, while Mondays and Fridays have 1.4% and 1.3% lower NO_2 pollution than a typical weekday. On Saturdays, NO_2 is 16% lower than the weekday averages, and on Sundays 24% lower.

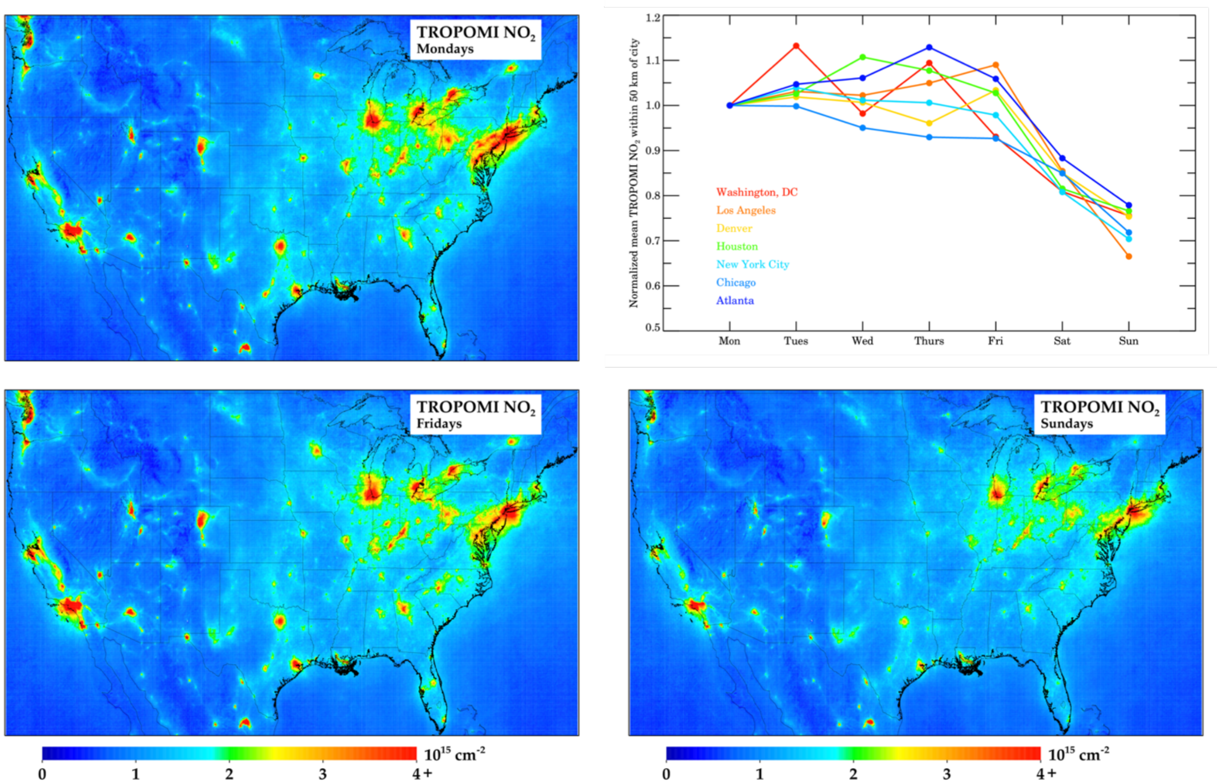

Figure 6. Weekly variations in column NO_2. (Top left) TROPOMI NO_2 during Mondays. (Bottom left) TROPOMI NO_2 during Fridays. (Top right) Weekly variation of TROPOMI NO_2 in 7 U.S. cities normalized to Mondays. (Bottom right) TROPOMI NO_2 during Sundays.

It is interesting to see the differences in the weekday patterns amongst the cities. In Chicago and Washington, D.C., column NO_2 is 10% lower on Fridays compared to earlier days in the week. Conversely, in Los Angeles and Denver, NO_2 is larger on Fridays as compared to previous days of the week. In Chicago and Washington D.C., we hypothesize that this may be an indication of teleworking on Fridays. Conversely, the cities with higher pollution on Fridays, are generally located in mountain valleys with stagnant winds – the valleys may be facilitating an accumulation of pollution during the week.

When analyzing the weekday/weekend differences, there should be some consideration for the difference in traffic patterns and general activity between weekends and weekdays. On weekends, traffic counts generally peak in the early afternoon, while on weekdays traffic counts peak in the evening, with a secondary peak in the early morning (de Foy, 2018). Since the satellite observation is acquired in the early afternoon, we suggest that the 24-hour averaged NO_X emissions difference between weekdays and weekends may be even greater than implied by the satellite data. The soon-to-be-launched TEMPO instrument, a geostationary satellite, will hopefully be able to better quantify the morning and evening differences of NO_X emissions (Chance et al., 2019; Penn & Holloway, 2020; Zoogman et al., 2017).

Hot vs. Warm Days

In Figure 7, we show the variation in column NO_2 as a function of the daily maximum 2-meter temperature (T2m-Max). Due to varying climates across the U.S. most cities do not have values for all temperature bins. In general, as temperatures increase, NO_2 decreases; this is primarily driven by $j(NO_2)$ which increases with stronger sunlight. When temperatures are >32°C, we observe a leveling with increasing temperature. This may be related to increasing anthropogenic NO_X emissions (Abel et al., 2017; He et al., 2013) at high temperatures despite a shorter NO_2 lifetime. This may also be driven by biogenic or natural causes, such as the faster dissociation of peroxy-acyl nitrates (PANs) or increased soil NO_X emissions (Rasool et al., 2019; Romer et al., 2018) at hot temperatures. The latter reasons are likely causing rural areas to observe increases in NO_2 as temperatures warm above 32°C. The temperature-driven stabilization of NO_2 at very high temperatures appears to hold for all cities except Chicago.

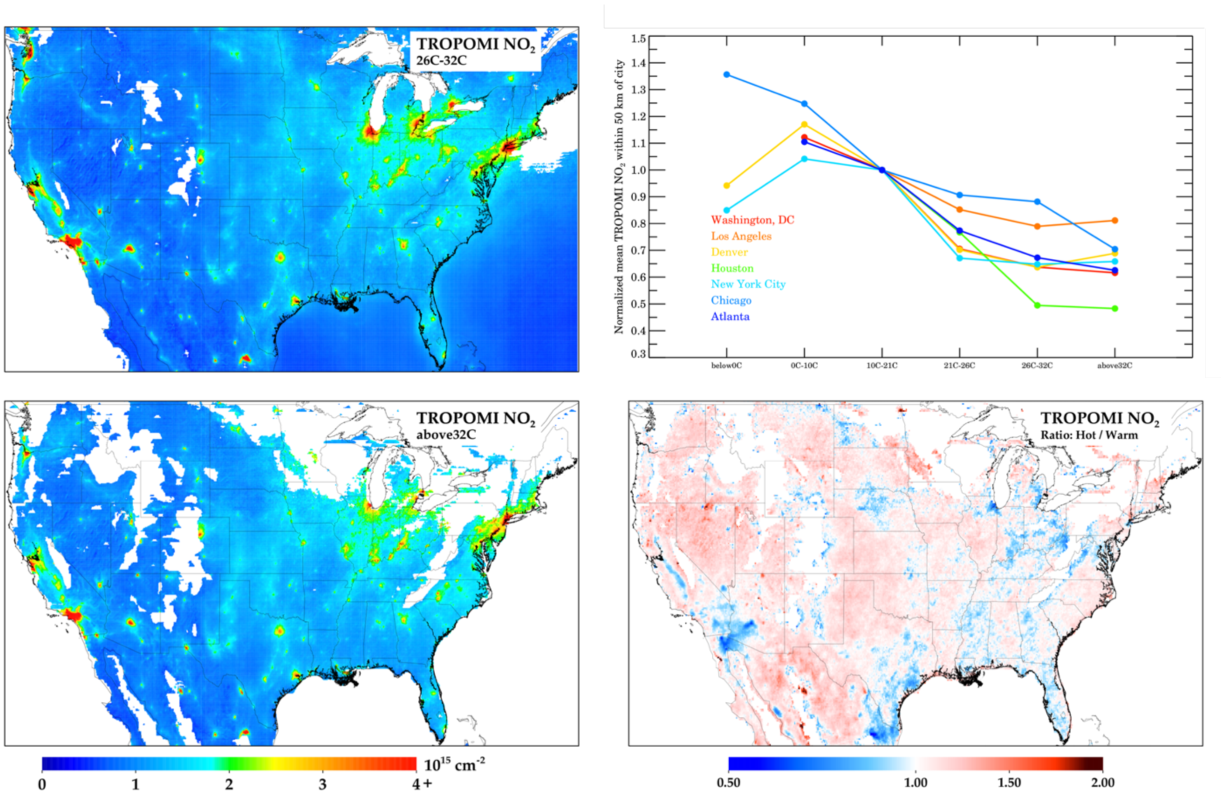

Figure 7. Temperature variations in column NO_2. (Top left) TROPOMI NO_2 when maximum daily 2-m temperature (T2m-Max) is between 26°C – 32°C (Warm; 80°F – 90°F); only areas were >10 valid pixels are shown. (Bottom left) TROPOMI NO_2 when T2m-Max is greater than 32°C (Hot; 90°F); only areas were >10 valid pixels are shown. (Top right) Temperature variation of TROPOMI NO_2 in 7 U.S. cities normalized to 10°C – 21°C (50°F – 70°F). (Bottom right) Ratio between bottom left and bottom right panel.

Relationship with $PM_{2.5}$

To understand the spatial pattern of NO_2 in comparison to $PM_{2.5}$, we compare TROPOMI annual averages of column NO_2 to estimates of surface-level $PM_{2.5}$ (VanDonkelaar et al., 2019). Both pollutants have generally short atmospheric lifetimes and often have similar regional patterns. In Figure 8, we depict the ratio between normalized TROPOMI NO_2 and normalized surface $PM_{2.5}$ using the equation below.

$$\frac{PM_{2.5}/\overline{PM_{2.5}}}{NO_2/\overline{NO_2}}$$

The red color in Figure 8 indicates that $PM_{2.5}$ is relatively larger than NO_2 and blue indicates that NO_2 is relatively larger than $PM_{2.5}$. There are instances, especially in cities, where $PM_{2.5}$ and

NO_2 are both greater than the CONUS mean, but that one pollutant is much larger than the mean and the other value is only slightly larger than the mean.

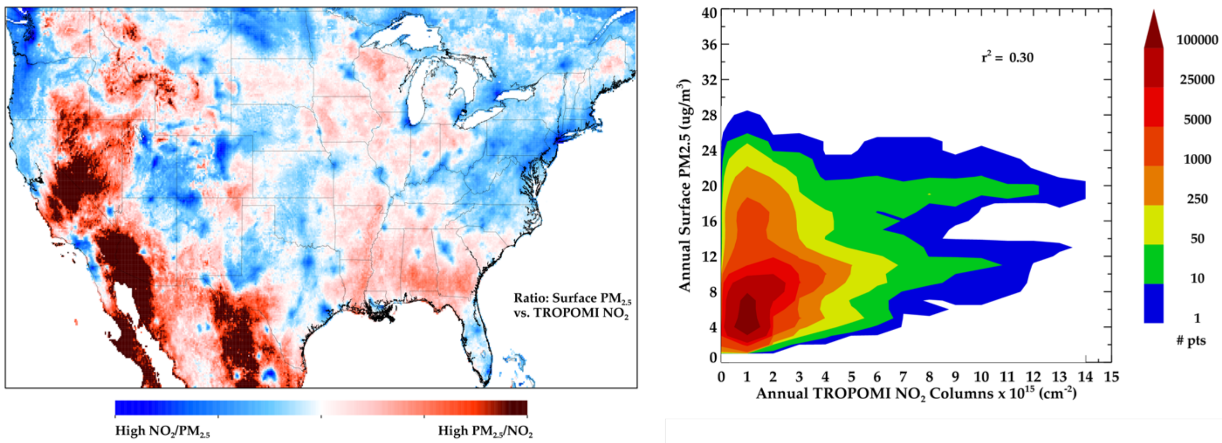

Figure 8. (Left) Ratio of oversampled 2019 TROPOMI NO_2 / 2016 Surface $PM_{2.5}$. (Right) Scatterplot of the two datasets. 2016 is latest year of the 0.01° × 0.01° $PM_{2.5}$ dataset (van Donkelaar et al., 2019) and is used for illustrative purposes. Spatial heterogeneities of annual $PM_{2.5}$ is likely similar between 2016 and 2019.

In major cities (e.g., New York City, Chicago, Los Angeles), NO_2 is more elevated from the mean CONUS concentration compared to $PM_{2.5}$. This is also true regionally in the Northeast and Pacific Northwest. Conversely, $PM_{2.5}$ is relatively elevated compared to the mean in four distinct rural CONUS regions: the desert Southwest, the Intermountain West, the Central Plains, and the Southeast. In the Southwest this is driven by dust. In the Intermountain West, this is likely driven by wildfires. In the Southeast and Central Plains, it is most likely driven by a combination of biogenic aerosols (e.g., secondary organic aerosols) and agricultural operations.

We then compare the NO_2 and $PM_{2.5}$ datasets using a scatterplot. We find low correlation between column NO_2 and surface $PM_{2.5}$ ($r^2 = 0.30$). At high TROPOMI NO_2 values, $PM_{2.5}$ is moderately elevated, but at low TROPOMI NO_2 values, there is a range of distribution of $PM_{2.5}$ with no correlation. This is in general agreement with studies showing that NO_2 hotspots are dominated by local and regional components, while $PM_{2.5}$ is dominated by regional and long-range components, with a lesser influence of local sources (Wang et al., 2020). Nevertheless, we find it important to demonstrate that TROPOMI NO_2 does not appear to be helpful in predicting surface $PM_{2.5}$ in the US.

Conclusions

This study investigates the capabilities of the Tropospheric Monitoring Instrument (TROPOMI) in observing the spatial and temporal patterns of NO_2 pollution in the Continental United States (CONUS). Here, we demonstrate that TROPOMI can capture fine-scale spatial heterogeneities in urban areas, such as hotspots related to airport/shipping operations and high traffic areas; this type of spatial precision cannot be matched by predecessor satellite instruments over short timescales (<1 year). We find that Saturday and Sunday concentrations are 16% and 24% lower respectively than during weekdays, with the caveat that diurnal emissions patterns vary among weekdays and weekends. We also analyze the effects of hot temperatures (>32°C) on NO_2 column amounts and find that column NO_2 is generally larger on the hottest days as compared to warm days (26°C - 32°C). Finally, we compare column NO_2 with estimates of surface $PM_{2.5}$ and find fairly poor correlation, suggesting that NO_2 and $PM_{2.5}$ are not well correlated in CONUS.

For this work, we rely on the operational TROPOMI NO_2 algorithm, which underestimates tropospheric vertical column NO_2 in urban areas. Previous studies suggest that this underestimate is due to the air mass factor (AMF) and ~5km pixel size which cannot resolve street-level variations in concentrations (Goldberg, Lu, Streets, et al., 2019; Griffin et al., 2019; Judd et al., 2019, 2020; Zhao et al., 2020); investigating the effects of the AMF bias on trends as well as investigating the effects of the pixels sizes will be the subject of future work. Also, there may be a clear-sky bias (Geddes et al., 2012) associated with any satellite retrieval, but the general spatial heterogeneities of NO_2 pollution, should be similar amongst all types of weather conditions, when averaged over long timeframes. Lastly, interpreting results from polar-orbiting satellite instruments such as TROPOMI, should be made with some caution due to the mid-day only data collection time. Work quantifying this bias has shown that NO_2 column measurements are lower and incrementally more spatially homogeneous in the afternoon than during the morning (Chong et al., 2018; Fishman et al., 2008; Herman et al., 2019; Knepp et al., 2015; Penn & Holloway, 2020; Tzortziou et al., 2015); it is likely that data from geostationary platforms such as TEMPO (Zoogman et al., 2017), GEMS (W. J. Choi, 2018), and Sentinel 4 (Timmermans et al., 2019), will be able to provide further insight on this time-of-day bias.

Because TROPOMI can observe and measure NO_2 increases attributed to relatively small sources, future work should be able to quantify emissions from small sources (e.g., industrial activities, small wildfires) that had previously gone undetected from predecessor space-based instruments. Furthermore, due to the instrument's excellent stability, precision, and spatial resolution, it is no longer necessary to average over 6+ months of data to gain a clear depiction of regional NO_2 abundances; instead monthly, weekly or even daily aggregations could suffice for many purposes. The examples presented here demonstrate how TROPOMI NO_2 satellite data can be advantageous for policymakers requesting information at high spatial resolution and short timescales, in order to assess, devise, and evaluate regulations. Future health impact assessment studies can use the high-spatial resolution capabilities of TROPOMI NO_2 to investigate disparities in traffic-related air pollution exposure and associated health effects between neighborhoods and population sub-groups within cities.

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