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Satellite Detection of NO_2 Distributions and Comparison with Ground-Based Concentrations

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Abstract

In this study we assess the capability of current-generation satellites to capture the variability of near-surface nitrogen dioxide (NO_2) monitoring data, with the goal of supporting health and regulatory applications. We consider NO_2 vertical column densities (VCD) over the United States from two satellite instruments, the Tropospheric Monitoring Instrument (TROPOMI), and Tropospheric Emissions: Monitoring of Pollution (TEMPO), and compare with ground-based concentrations as measured by the EPA's Air Quality System (AQS) monitors. While TROPOMI provides a longer-term record of assessment (2019-2023), TEMPO informs diurnal patterns relevant to evaluating peak NO_2. We analyze frequency distributions and quantify their similarity using the Jensen-Shannon Divergence (JSD), where smaller values indicate better agreement. Satellite and ground monitor NO_2 distributions are most similar away from major roads, as indicated by the JSD of 0.008 calculated for TROPOMI and ground monitors at non-roadways, compared with a JSD near interstates of 0.158 and a JSD near highways of 0.095. Seasonal analysis shows the most similarity in distributions in winter, with a JSD of 0.010, and the most difference in summer, with a JSD of 0.035. Across seasons and monitor locations, TEMPO consistently has a lower or similar JSD as TROPOMI, with TEMPO JSDs ranging from 0.005 to 0.151 and TROPOMI JSDs ranging from 0.012 to 0.265. TEMPO's agreement with

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monitors in both December 2023 and July 2024 is found to be best around midday, with non-road monitors' JSD in July as low as 0.008 at 16 UTC (~11am LT).

1 Introduction

The frequency distribution of ambient pollutants in urban areas has long been recognized as a useful metric for comparison with health-based thresholds, and to assess the effectiveness of emission controls. Early studies found pollutant concentrations in urban areas to be approximately lognormally distributed (Knox and Lange, 1974; Pollack, 1975; Venkatram, 1979) and isolated point sources better described by exponential distributions (Venkatram, 1979). The distributional lens also bears relevance to advanced health and regulatory assessment (Chowdhury et al.,2021; Mondal et al., 2021). In this study we evaluate the capability of current-generation satellites to capture the variability of near-surface nitrogen dioxide (NO_2) monitoring data, with the goal of supporting health and regulatory applications.

Nitrogen dioxide (NO_2) is a gas released through high temperature combustion processes such as the burning of fossil fuels (Lee et al., 1997; Richter et al., 2005), with on-road vehicles, power plants, and industrial processes representing the largest anthropogenic sources in the United States (U.S.; van der A et al., 2008). Exposure to elevated levels of NO_2 has been linked to respiratory and cardiovascular diseases (Mills et al., 2015; Urbanowicz et al., 2023; Meng et al., 2021), especially asthma in children (Mölter et al., 2014; Anenberg et al., 2022; Achakulwisut et al., 2019), as well as premature mortality (Camilleri et al., 2023; Hales et al., 2021; Huangfu and Atkinson, 2020), and other diseases (Xia et al., 2024; Bai et al., 2018). NO_2 plays a critical role in the formation of ozone, which also causes respiratory health problems and is harmful to ecosystems (Grulke & Heath, 2019; Sillman, 1999). It is also a precursor to nitrate (Behera & Sharma, 2012), a type of fine particulate matter ($PM_{2.5}$), which can penetrate deep into the lungs and exacerbate respiratory and heart conditions (Sangkham et al., 2024; Sharma et al., 2020), as well as cause premature death (Orellano et al., 2020; Thangavel et al., 2022).

The EPA Air Quality System (AQS) contains hourly NO_2 measurements from ground-based monitors, providing high temporal resolution data that are critical for assessing compliance with the U.S. National Ambient Air Quality Standards (NAAQS). There are two NAAQS related to NO_2: one for annual average concentration, set at 53 ppb, and one based on peak 1-hour

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concentrations, set at 100 ppb, based on the 3-year average of the 98th percentile of the yearly distribution of 1-hour daily maximum NO_2 concentrations (EPA, 2010). Enforcement of these standards relies on data from AQS NO_2 monitors, a network that includes 431 monitors as of 2024. Because NO_2 has a relatively short atmospheric lifetime, typically ranging from a few hours to a day depending on meteorological conditions (Lange et al., 2022; Liu et al., 2021), ground monitors are expected to capture local conditions (Wang et al., 2020).

Several studies have highlighted the potential for satellite NO_2 data to supplement ground-based networks (Duncan et al., 2014; Lee & Koutrakis, 2014). Due to its radiative characteristics, NO_2 may be observed by satellites during daylight hours (Boersma et al., 2018; Van Geffen et al., 2020; Veefkind et al., 2012), and NO_2 has emerged as one of the most air-quality-relevant pollutants from satellites (Holloway et al., 2021). Some of the first studies done comparing ground-based NO_2 to satellite VCDs (Lamsal et al., 2014; Lamsal et al., 2015; Zhang et al., 2018) used the Ozone Monitoring Instrument (OMI, 13 km × 24 km; Levelt et al., 2006). Annual OMI and surface NO_2 trends in the U.S. show that OMI usually overestimates the surface trends by ~3.7% each year (Zhang et al., 2018). With the 2017 launch of the Tropospheric Monitoring Instrument (TROPOMI; Boersma et al., 2018; Van Geffen et al., 2020; Veefkind et al., 2012), new opportunities arose for analyzing column-to-surface agreement at a higher resolution (3.5 km x 5.5 km) (Goldberg et al., 2021; Griffin et al., 2019; Kim et al., 2024; Yu & Li, 2022; Dressel et al., 2022; Goldberg et al., 2024; H. J. Lee et al., 2023).

While advanced methods exist to calculate near-surface NO_2 explicitly (Ahmad et al., 2024; Kim et al., 2021; Shetty et al., 2024; Virta et al., 2023), there is also a strong interest in the utilization of satellite vertical column density (VCD) to directly infer NO_2 concentrations analogous to ground-based monitors (Kim et al., 2024; Lamsal et al., 2014; Griffin et al., 2019; Yu & Li, 2022; Zhang et al., 2018; Lamsal et al., 2015; Goldberg et al., 2021; Dressel et al., 2022; Goldberg et al., 2024; Harkey & Holloway, 2024; Bechle et al., 2013; H. J. Lee et al., 2023; Xu & Xiang, 2023). This study extends these prior assessments of NO_2 column-to-surface agreement, where we focus on frequency distributions to capture the net impact of day-to-day variability.

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Past studies comparing surface and satellite NO_2 have found temporal correlation of daily values at individual sites ranging from r=0.61 to r=0.69 (Lamsal et al., 2014; Lamsal et al., 2015), monthly and seasonal values at individual sites ranging from r=0.67 to r=0.90 (Griffin et al., 2019; Yu & Li, 2022; Harkey & Holloway, 2024; Dressel et al., 2022; Xu & Xiang, 2023; Lamsal et al., 2015), and annual average values at sites ranging from r=0.68 to r=0.93 (Zhang et al., 2018; Lamsal et al., 2015; Goldberg et al., 2021; Kim et al., 2024; Bechle et al., 2013; H. J. Lee et al., 2023). Here, r refers to the Pearson correlation coefficient, which measures the strength and direction of a linear relationship between variables. In some cases, these comparisons adjusted column values to the surface (e.g. Lamsal et al., 2014) and/or adjusted ground-monitors to reduce the error in chemiluminescent detection of NO_2 (e.g. Lamsal et al., 2015; Bechle et al., 2013). Using similar methods, TROPOMI tends to show better agreement with annual AQS NO_2 than does OMI, e.g. r=0.81 using TROPOMI (Goldberg et al., 2015) versus r=0.68 from OMI (Lamsal et al., 2015). Off-road AQS monitors tend to show better agreement with satellite data than near-road AQS monitors, e.g. r = 0.81-0.87 at non-near-road sites versus r = 0.64-0.74 at near-road sites (Kim et al., 2024). The underestimation of estimated near-surface NO_2 near roads and localized sources is a recurring issue in OMI and TROPOMI NO_2 VCDs (Dressel et al., 2022; Goldberg et al., 2024; Ialongo et al., 2020).

The relationship between surface NO_2 and column abundance is influenced by physical and chemical processes, many of which have seasonal components. In winter, shallow boundary layers trap pollutants near the surface, leading to higher surface concentrations and increasing surface-to-column agreement (Harkey et al., 2015). In summer, higher temperatures and increased sunlight accelerate photochemical reactions, converting NO_2 into ozone and other secondary pollutants, and decreasing surface-to-column agreement (Boersma et al., 2009). Seasonal changes in emissions, such as high building-heating emissions in winter, and high power plant emissions in summer (Frost et al., 2006; Levinson & Akbari, 2010) interact with atmospheric processes causing an increase in NO_2 column abundance in winter in four-season climates (Shah et al., 2020). Processes affecting the sources and sinks of NO_2 at the surface and through the vertical column can also lead to temporal lags, with peak surface NO_2 preceding peak column NO_2 in the mornings (Harkey et al. 2024).

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Frequency distributions capture the variability, extremes, and patterns of pollutant abundance, relevant to air quality standards, pollution trends, and the effectiveness of emission control measures. For example, Mondal et al. (2021) used frequency distributions of ground-based monitors to examine changes in air quality across Delhi and Kolkata during COVID-19 lockdown phases, showing how reduced human activity led to shifts in pollutant levels. We extend this line of analysis by comparing NO_2 distributions across multiple dimensions with TROPOMI and include time-of-day and resolution-dependence of results using data from the Tropospheric Emissions: Monitoring of Pollution (TEMPO; Chance et al., 2019; Naeger et al., 2021; Zoogman et al., 2017). TEMPO provides daytime hourly observations of NO_2 over North America and finer spatial coverage—approximately 2.1 km by 4.5 km at its center.

The Jensen-Shannon Divergence (JSD) is a robust metric for comparing probability distributions that is used within a wide variety of fields, including machine learning (Thiagarajan & Ghosh, 2024; Saurette et al., 2023; Tsigalou et al., 2021; Melville et al., 2005), data science (Toledo et al., 2022; Zhao et al., 2024), biology (Yan et al., 2021; Jones et al., 2023; Ahmed et al., 2023), and meteorology (Kibirige et al., 2023). In environmental research using satellite data, the JSD has shown that the Mangrove Forest Index (MFI) from Sentinel-2 imagery outperforms traditional vegetation indices in distinguishing submerged mangrove forests (Jia et al., 2019). In air quality, JSD has been used to compare modeled and measured $PM_{2.5}$ (Yang et al., 2024), and to compare an air quality index (AQI) with measurements of specific air pollutants (Wang & Zhang, 2022). We utilize the JSD to quantify the similarity between satellite and monitored NO_2 distributions, applying this well-established metric to satellite-derived air quality evaluation.

In this work, we consider: (1) How do the distributions of satellite NO_2 VCD compare with those for near-surface NO_2? (2) To what degree does new hourly data from TEMPO improve the agreement between surface and space based NO_2 distributions? For both questions, we consider spatial variability, especially proximity to roadways, and temporal variability including seasonality and diurnal variability. By considering the ability of satellites to capture peak NO_2 values in a comparable distribution to surface data, we consider how satellite VCDs can support air quality management, improve health impact analysis, and inform air pollution monitor siting.

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2 Data and Methods

In this study, we evaluate the ability of two satellite instruments, TROPOMI and TEMPO, to capture the spatial and temporal variability in NO_2 surface concentration distributions across the continental United States (CONUS), as measured by AQS monitors. By comparing the coefficient of variation (CV) and Jensen-Shannon divergence (JSD) between satellite and monitor data, we aim to assess the alignment between the datasets.

2.1 EPA Surface Monitor Data

The EPA Air Quality System (AQS) was used to access NO_2 monitor data for the years 2019 through 2023 from all available sites in CONUS during this time period (N=503). Most monitors use a chemiluminescence method, where the amount of NO_2 that is converted to NO is measured by a molybdenum oxide converter (Fontijn et al., 1970). The converter also reacts with other oxidized nitrogen compounds such as nitric acid (HNO_3) and peroxyacetyl nitrate (PAN) to form NO (Dunlea et al., 2007; Steinbacher et al., 2007), which can lead to an overestimation of NO_2. Corrections for this bias have been applied when comparing with satellite observations (e.g. Cooper et al., 2020; Lamsal et al., 2015; Li et al., 2021). Uncorrected AQS NO_2 has been used for determining compliance with the NAAQS and for health assessments, which is the approach we take here, consistent with prior studies focused on regulatory relevance (Novotny et al., 2011; Penn & Holloway, 2020; Harkey and Holloway, 2024; Goldberg et al., 2021; Kim et al., 2024; Duncan et al., 2013; Qin et al., 2019). More recently, some NO_2 monitors have been added to the network which measure "true NO_2" using Cavity Attenuated Phase Shift Spectroscopy (CAPS, Kebabian et al., 2005). These monitors are expected to be more representative of ground-level NO_2 concentrations and have less overestimations since they directly measure NO_2 and no other species (Ge et al., 2013). Some of the monitors used in this study use CAPS methodology to measure NO_2. We discuss the comparison of CAPS versus traditional NO_2 monitors in results Sect. 3.1.

Hourly AQS measurements at 13:00 and 14:00 local time (LT) were averaged to align with the TROPOMI overpass of ~13:30 LT. Hourly AQS measurements from 12:00 GMT to 23:00 GMT are compared with hourly TEMPO data for daylight hours. For both the TROPOMI and TEMPO analyses, AQS data are filtered to ensure consistency with satellite data availability. As a result

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of filtering monitoring data for TROPOMI and TEMPO separately, the subsets of monitor data available for comparison with each instrument differ, even for the same time periods.

2.2 TROPOMI Data

The Tropospheric Monitoring Instrument (TROPOMI) is on board the Copernicus Sentinel-5 Precursor satellite which has a daily, local overpass time of ~13:30 LST (Veefkind et al., 2012). Currently, the highest resolution of TROPOMI is 3.5 km by 5.5 km at nadir which has increased from 3.5 km by 7.0 km since August 6th, 2019. Daily TROPOMI NO_2 data for the years 2019 through 2023 were allocated to a 4 km x 4 km grid over CONUS using the Wisconsin Horizontal Interpolation Program for Satellites (WHIPS; Harkey et al., 2015, 2021; Harkey and Holloway, 2024; Penn and Holloway, 2020). Using WHIPS, we also remove data with quality flag lower than 0.75. Each monitor location was compared with the 4 km x 4 km gridded TROPOMI value in the corresponding grid cell. December 2023 and July 2024 4 km x 4 km TROPOMI NO_2 data were also collected for each of the monitors for comparison with TEMPO data.

2.3 TEMPO Data

The TEMPO instrument launched onboard the Intelsat 40e mission (NASA, 2024), a geostationary satellite, on April 7, 2023. TEMPO provides hourly measurements of atmospheric pollutants over North America (Chance et al., 2019; Naeger et al., 2021; Zoogman et al., 2017). TEMPO achieves a spatial resolution of approximately 2.1 km in the north-south direction and 4.5 km in the east-west direction at the center of its Field of Regard (FOR), centered around 36.5° N and 100° W (Chance et al., 2019). The TEMPO Level-3 (L3) NO_2 data (Suleiman, 2024) used in this study were accessed through NASA's EarthData Search portal.

In order to synchronize TEMPO and ground-based hourly measurements, TEMPO timestamps were rounded to the nearest hour, with mid-hour values rounded up. All files within each rounded-hour group were averaged, producing a single NO_2 value per hour per day. Only TEMPO observations with a main data quality flag of 0 and cloud fraction at or less than 0.2 were retained, in line with TEMPO documentation guidelines (NASA Langley Research Center, 2024).

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For the comparison with TROPOMI, the UTC equivalents of 1 pm and 2 pm LT were determined for each time zone based on the latitude and longitude of each monitor location. TEMPO NO_2 values corresponding to these calculated UTC hours were averaged to align with the TROPOMI overpass time (~13:30 LST). Similarly, for ground-based measurements, the monitor data were filtered to include only values corresponding to 1 pm and 2 pm LT and then averaged.

2.4 Monitor Classification

To classify the monitors by roadway proximity, the state-level Census Bureau's 2021 TIGER/Line shapefiles for Primary and Secondary Roads were combined to form a comprehensive dataset for the CONUS domain.

To evaluate how TROPOMI and ground-based monitor NO_2 values vary by proximity to a road, monitors were also assigned to different groups based on their distance from a road (≤20-m, 20 to 50-m, 50 to 300-m, 300-m to 1mi, and >1mi), where buffer distances are calculated from the road shapefiles (Figure S2). There were 9 monitors that were 20 meters or less away from a road, 66 between 20 and 50 meters from a road, 108 between 50 and 300 meters, 219 between 300 meters and 1 mile, and 101 that were greater than 1 mile from a road.

Roads were also classified into three categories: (1) interstates, (2) highways, and (3) other roads, based on their route type code (RTTYP) values. Where monitors are considered as representing a roadway category, we followed the criteria of the EPA Near-Road-Network (Gantt et al., 2021; Kim et al., 2024), to merge monitor locations with road buffers, considering the 50-m buffer recommended by EPA, as well as a less restrictive 300-m buffer. In each case, monitors inside the buffer of a particular roadway type were classified as representing that category. If a monitor fell within multiple buffers, it was assigned the classification of the largest road type. Monitors not falling within any buffers were classified as "non-roadway."

Using the 50-m buffer, 58 monitors were classified as "interstate," 17 as "highway," and 428 as "non-roadway" (Figure S1; no monitors classified as "other roads"). Using the 300-m buffer, 91 monitors were classified as "interstate," 90 as "highway," 320 as "non-roadway," and 2 as "other roads." Since there were no monitors classified as "other roads" for the 50-m buffer, this category is excluded from the analysis.

2.5 Data Analysis

The coefficient of variation (CV) was calculated for ground-level monitor data and for satellite data. This metric was used to compare the relative variability of NO_2 between satellite and ground-level data despite different measurement units (Aerts et al., 2015). CV is defined as the ratio of the standard deviation (σ) to the mean (μ) of the data:

$$CV = \left(\frac{\sigma}{\mu}\right) \times 100$$

The Jensen-Shannon Divergence (JSD) quantifies the similarity between the distributions of NO_2 from satellite and ground-level monitors despite the different measurement units (Menéndez et al., 1997). To calculate JSD, each dataset was binned, with a bin size of 1 ppb or 1 x 10^{15} molecule/cm^2, ranging from 0 to 40 ppb or 40 x 10^{15} molecule/cm^2, with an additional bin for values exceeding 40 ppb or 40 x 10^{15} molecule/cm^2. Binned data were then normalized to form probability distributions. The divergence was calculated as:

$$JSD(P,Q) = \frac{1}{2}[D_{KL}(P||M) + D_{KL}(Q||M)]$$

where P and Q represent the probability distributions from the monitor and satellite data, respectively, and M is the average of P and Q. The divergence D_{KL} is the Kullback-Leibler divergence between each distribution and their mean (Clim et al., 2018). JSD values range from 0 to 1, with lower values indicating greater similarity between the satellite and monitor distributions. In general, a JSD < 0.1 indicates very good alignment, 0.1 ≤ JSD < 0.3 indicates moderate alignment, and JSD ≥ 0.3 (Kibirige et al., 2023) indicates poor alignment.

3 Results

To evaluate the agreement between satellite and monitored NO_2 distributions, we consider the impact of monitor location using TROPOMI; impact of season using TROPOMI; the comparison of distributions between TROPOMI and TEMPO; and the impact of time-of-day using TEMPO.

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3.1 Alignment of TROPOMI NO_2 Distributions with Surface NO_2 Distributions

Figure 1 illustrates the distribution of NO_2 levels measured by AQS ground-based monitors and TROPOMI observations as a function of distance from roadways. For both data sources, mean, peak, and minimum NO_2 are all highest in the 20 – 50m distance category (the second closest near-road category). NO_2 abundance decreases as distance-to-road increases, and to a lesser extent as distance-to-road decreases. The somewhat lower abundance ≤ 20 m vs. the 20 – 50 m category may be due to the speciation of NO_X, where NO is more abundant and converts to a higher fraction of NO_2 as distance-to-road increases (Kimbrough et al., 2017). Mean monitored NO_2 is 6.85 ppb at ≤ 20 m, 10.47 ppb at 20 – 50 m, 4.53 ppb at 50 – 300 m, 3.53 ppb at 300 m – 1 mi, and 2.76 ppb at > 1 mi. Mean TROPOMI NO_2 is 3.38 x 10^{15} molecules/cm^2 at ≤ 20 m, 4.21 10^{15} molecules/cm^2 at 20 – 50 m, 3.00 x 10^{15} molecules/cm^2 at 50 – 300 m, 3.63 x 10^{15} molecules/cm^2 at 300 m – 1 mi, and 3.04 x 10^{15} molecules/cm^2 at > 1 mi. Monitor values show a higher sensitivity to roadway proximity, where the highest mean monitored concentration is 379% of the lowest mean concentration, compared to TROPOMI where the highest mean VCD is 138% of the lowest mean VCD.

Monitored NO_2 levels drop over 50% at ~50 m from the roadway (based on change in the mean, upper 2.5 interquartile range, IQR, and the upper 1.5 IQR), a finding that compares with 31% reduction in NO_2 between 20m and 300m from Kimbrough et al. (2017), as well as other studies that identify a decrease in NO_2 at further distances (Karner et al., 2010; Richmond-Bryant et al., 2017). TROPOMI VCDs also show the greatest change with roadway distance at ~50 km, but by less than 30% (based on change in the mean, upper 2.5 IQR, and the upper 1.5 IQR).

Just as total NO_2 abundance, from both monitors and satellite, is highest at distances of 20-50 m from the roadway, the range of daily values is also widest for the 20 – 50 m range and smallest at the > 1 mi range. Monitored values have a standard deviation of 8.24 ppb in the 20 – 50 m range, and a standard deviation of 3.44 ppb in the > 1 mi range. The distribution of satellite data does not vary as much in size across roadway locations, with a standard deviation of 3.90 x 10^{15} molecules/cm^2 for the 20 – 50 m range and 3.39 x 10^{15} molecules/cm^2 for the > 1 mile range. In the 20 – 50 m range, the upper IQR of AQS NO_2 is 38% higher than the mean. TROPOMI shows less variability than the monitors, with the 20 – 50 m upper IQR 16% higher than the mean. As distance from the roadway increases, the distributions of data from ground and satellite become

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more comparable. In the > 1 mile range, the upper IQR of monitor NO_2 is 30% higher than the mean and the upper IQR of satellite data is 15% higher than the mean. The ranges show more similarity at greater distance from the roadway, but even at distances of > 1 mile, the range of monitored values exceeds the range of satellite VCDs. These patterns agree with Kim et al. (2024), who found that surface monitors show better agreement with TROPOMI further from major roads.

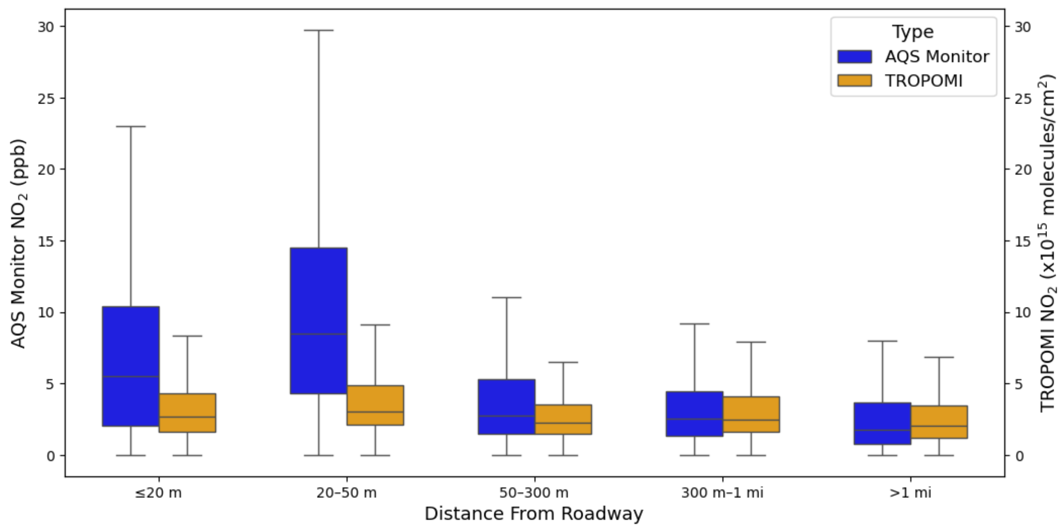

Figure 1. Box plots show median and interquartile ranges of NO_2 as measured by AQS monitors (blue) and TROPOMI (orange) across various distances from roadways, with the whiskers extending to the 1.5 IQR range. No outliers are shown. The left y-axis represents AQS monitor values in parts per billion (ppb), and the right y-axis represents TROPOMI NO_2 values in 10^{15} molecules per cm^2. The distance categories from the roadway include ≤20m, 20-50m, 50-300m, 300m-1mi, and >1mi.

To consider the shape of monitored and satellite NO_2 distributions, we consider the effect of season in Fig. 2. The winter distributions (Figure 2a, calculated from December, January, and February data) exhibit the longest tails and highest NO_2 values. In winter the 90th percentile of monitoring data is 14.80 ppb and the 90th percentile of TROPOMI data is 10.93 x 10^{15} molecules/cm^2. In summer (Figure 2c, June, July, and August) the distributions exhibit the shortest tails, and the lowest NO_2 values (90th percentile from monitors = 9.00 ppb, 90th

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percentile from TROPOMI = 4.57 x 10^{15} molecules/cm^2). The fall (Figure 2d, September, October, and November) and spring (Figure 2b, March, April, and May) distributions show behavior in between winter and summer. The higher NO_2 values in winter from monitor and TROPOMI data are attributed to reduced photochemical activity in winter leading to longer NO_2 lifetimes (Harkey et al., 2015; Boersma et al., 2009; Shah et al., 2020).

The highest percent frequencies for the monitor and TROPOMI distributions generally occur within the 1–2 ppb or 1–2 x 10^{15} molecules/cm^2 bin. However, the winter TROPOMI distribution peaks in the 2–3 x 10^{15} molecules/cm^2 bin with a percent frequency of 18.14%, compared with winter monitor highest frequency of 14.33%. The highest percent frequency in spring from TROPOMI is 30.39% versus monitor 24.15%; in summer TROPOMI is 34.35% versus monitor of 24.68%; in fall TROPOMI is 24.90% versus monitor of 18.89%. These results indicate that TROPOMI consistently records higher peak frequencies than the monitors, whereas monitors consistently show a wider distribution.

Figure 2 provides a seasonal breakdown of the coefficient of variation (CV) and Jensen-Shannon divergence (JSD) for both monitor and TROPOMI data across all monitors. Summer exhibits the highest variability in monitored NO_2 concentrations (CV = 127.99%), but the lowest variability in satellite observations (CV = 78.00%). The highest variability in TROPOMI occurs in winter (CV = 103.51%), similar to the variability from monitor data (CV = 104.48%). Satellite CVs generally follow a similar pattern to that of the monitors, though the overall variability is lower for satellite data across seasons.

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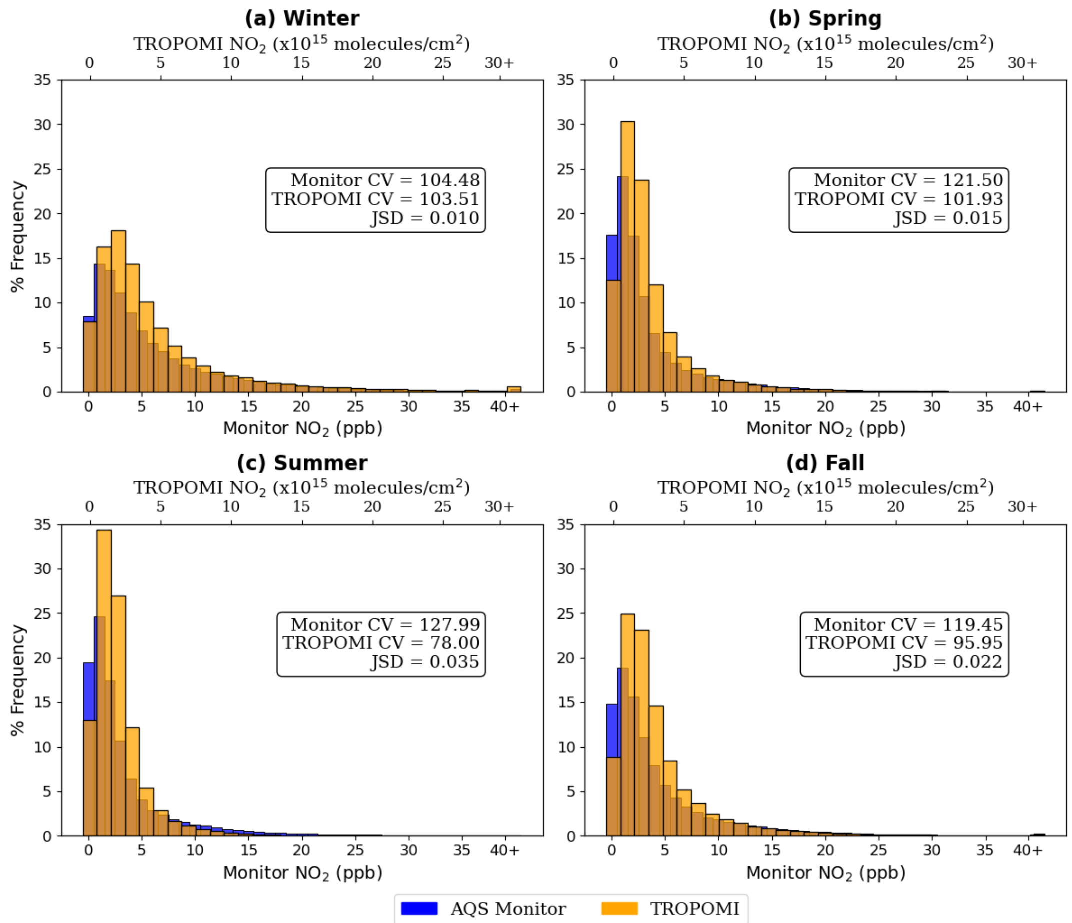

Figure 2. Seasonal frequency distributions of 2019-2023 NO_2 as measured by AQS ground-based monitors (blue) and TROPOMI (light orange) data for four seasons: a) winter, b) spring, c) summer, and c) fall. The x-axes indicate the range of NO_2, with the primary, lower x-axis showing monitor NO_2 concentrations in parts per billion (ppb) and the secondary, upper x-axis showing TROPOMI NO_2 VCD in 10^{15} molecules per cm^2. The boxes show the Coefficient of Variation (CV; %) and Jensen Shannon Divergence (JSD) for each season.

This reduced variability in satellite observations can likely be attributed to the vertical mixing reflected in satellite retrievals, as well as horizontal spatial averaging reflected in satellite data versus point-based NO_2 that are captured by ground monitors. This finding is consistent with previous studies that highlight the spatial averaging nature of satellite-based measurements,

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which integrate NO_2 amounts over a larger area than the point-based monitors (Ialongo et al., 2020).

Across all seasons shown in Fig. 2, JSD values are all low (< 0.1), indicating that TROPOMI may be good at predicting surface NO_2 across seasons. The alignment is strongest in winter (JSD = 0.010), while the divergence is highest in summer (JSD = 0.035), meaning the monitors and TROPOMI align best when the NO_2 lifetime is long in the colder months, and align the worst when the NO_2 lifetime is short in the warmer months.

Across seasons, we find that CAPS or "true NO_2" monitors tend to have slightly worse alignment with TROPOMI than traditional, chemiluminescence monitors. Out of the monitors used in this study, 102 were identified as CAPS monitors, and 401 as traditional monitors. In winter, CAPS monitors have a JSD of 0.027 and traditional monitors a JSD of 0.009. In summer, CAPS monitors have a JSD of 0.078 and traditional monitors a JSD of 0.03. With all seasons combined, CAPS monitors have a JSD of 0.047 and traditional monitors have a JSD of 0.016.

Table 1 shows the CV and JSD for both monitor and satellite data from 2019 through 2023, aggregated across all seasons and separated by monitor classification (interstate, highway, and non-roadway), where roadway monitors are classified as being within 50 meters (Table 1a) or 300 meters (Table 1b) of a road. For the 50-m buffer (Table 1a), the coefficient of variation for ground-based monitor data increases progressively from interstate monitor locations to non-roadway locations, with interstate monitors exhibiting the lowest variability (CV = 75.07%) and non-roadway monitors showing the highest variability (CV = 118.17%). This indicates that NO_2 concentrations measured by ground monitors in interstate areas are more consistent compared to non-roadway regions. This pattern is mirrored in the satellite data, with CV values ranging from 91.62% for highway monitors to 106.16% for non-roadway monitors. These patterns suggest that regular emissions play a larger role in determining near-road NO_2, where non-road areas vary with changes in wind patterns and the chemical environment.

For highway monitors, the CVs of satellite (CV = 91.62%) and monitor data (CV = 96.27%) are similar, indicating that TROPOMI performs similarly to ground monitors in capturing NO_2 variability along highways. Near interstates, TROPOMI (CV = 92.60%) may capture more variability than the ground-based measurements (CV = 75.07%), a finding that contrasts with Fig. 1, where TROPOMI shows a narrower range of NO_2 values across all distances. This

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difference could stem from the fact that the interquartile ranges in Fig. 1 measure the spread of absolute values, while the coefficient of variation accounts for variability relative to the mean. Together, these metrics reveal that TROPOMI may not fully capture localized extremes (narrower IQR) but still captures more relative variability in pollution near interstates than monitors (higher CV).

	Road Type	**Monitor CV**	**TROPOMI CV**	**JSD**	**# of Monitors**
a) 50-m Buffer	Interstate	75.07	92.60	0.158	58
	Highway	96.27	91.61	0.095	17
	Non-roadway	118.17	106.16	0.009	428
b) 300-m Buffer	Interstate	77.20	91.014	0.133	91
	Highway	135.76	92.31	0.017	90
	Non-roadway	116.23	108.43	0.008	320

Table 1. Coefficient of variation and Jensen-Shannon divergence for all seasons combined at interstate, highway, and non-roadway monitors 2019-2023 for the 50-m and 300-m roadway buffers.

The key differences seen within the JSD across the three monitor classifications are also present in the percent frequency distributions of NO_2 measured by ground-based monitors and TROPOMI (Figure S3), with interstate monitors having the lowest alignment (JSD = 0.158), highway monitors having better alignment (JSD = 0.095), and non-roadway monitors having the best alignment (JSD = 0.009). The strong alignment between TROPOMI and monitor distributions in non-roadway regions is consistent with previous studies (Dressel et al., 2022; Kim et al., 2024; Ialongo et al., 2020). This close alignment may be due to the relatively lower NO_2 concentrations, which TROPOMI captures more accurately compared to regions with higher emissions. These findings further align with previous work showing that TROPOMI tends to underestimate NO_2 in high-pollution areas (such as interstates and highways) but slightly overestimates in areas of lower pollution, such as rural areas (Dressel et al., 2022; Ialongo et al., 2020; Goldberg et al., 2024).

Due to the large jump in NO_2 levels seen within Fig. 1 in the 50-300m category, we compare the 50-meter buffer roadway classifications (Figure S3; Table 1a) with the 300-meter buffer

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classifications (Figure S4; Table 1b). Notable differences emerge between distributions, particularly in the highway category, where 73 monitors are added to the highway distribution (increasing from 17 to 90 monitors; Table 1) due to the larger buffer. The alignment between monitor data and TROPOMI observations is significantly improved within the 300-meter buffer near highways. This improvement in alignment is likely due to the decay of NO_2 with increasing distance from the road (Karner et al., 2010; Kimbrough et al., 2017; Richmond-Bryant et al., 2017). Consequently, the lower surface NO_2 concentrations observed at 300 meters are better captured by TROPOMI. This is reflected in Table 2, which shows a substantial reduction in the JSD for highway monitors, from 0.095 in the 50-meter buffer to 0.017 in the 300-meter buffer (an 82% increase in alignment at the 300-meter buffer).

The differences observed in the highway category with the 300-meter buffer may be present since the distribution includes 73 more monitors than the 50-meter buffer, capturing lower NO_2 amounts that are more aligned with TROPOMI's observations. On the other hand, the interstates category exhibits less noticeable change, with only 33 additional monitors in the 300-meter buffer distribution (increasing from 58 in the 50-meter buffer, Table 1a; to 91 in the 300-meter buffer, Table 1b). This suggests that the monitors added in the 300-meter buffer for interstates measure NO_2 levels similar to those already captured in the 50-meter buffer, resulting in little change to the overall distribution.

These results indicate that TROPOMI follows the trend of NO_2 decreasing with increasing distance from roadways that ground-based monitors record, and TROPOMI captures surface concentrations best in winter and at 300+ meters away from the traffic source.

3.2 Column-Column Daily Alignment

Figure 3 shows the distributions of NO_2 as measured by AQS ground-based monitors (filtered to match valid TROPOMI and TEMPO data), TROPOMI, and TEMPO, separated by road classifications (interstates, highways, and non-roadways) for December 2023 and July 2024. The monitor data in each comparison differs due to the data filtering (see Sect. 2.2 and 2.3). The comparison of frequency distributions reveals how well TEMPO and TROPOMI capture the wide range of ground-based monitor readings across these classifications and time periods.

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In December 2023, TEMPO (JSD = 0.007) and TROPOMI (JSD = 0.021) across road classifications show distinct patterns in their ability to represent NO_2 distributions across road classifications. Near interstates TEMPO shows a 90th percentile at 18.34 x 10^{15} molecules/cm^2 where the TROPOMI 90th percentile is 11.27 x 10^{15} molecules/cm^2. TEMPO aligns more closely with monitor distributions with a JSD of 0.066 compared to the TROPOMI JSD of 0.145 (Figure 3). TEMPO has 21.42% of data points above 11 x 10^{15} molecules/cm^2 for interstate values in December, whereas TROPOMI appears to underestimate the frequency of higher NO_2 levels more, with a cumulative frequency of 10.53% above that threshold. Near highways, the TEMPO 90th percentile is 14.70 x 10^{15} molecules/cm^2 compared to TROPOMI with a 90th percentile of 10.06 x 10^{15} molecules/cm^2. The JSD for TEMPO is 0.049 and TROPOMI is 0.125 for highway monitors, indicating that TEMPO has much better alignment on highways (Figure 3). For non-roadway locations, both instruments show very good alignment (TEMPO JSD = 0.005; TROPOMI JSD = 0.012; Figure 3) with the monitor data distributions, but with TEMPO again being slightly better.

In July 2024, the patterns show greater divergence across road classifications (TEMPO JSD = 0.027; TROPOMI JSD = 0.049) between the satellite observations and ground-based monitor data compared to the December 2023 distributions. Near interstates, the TEMPO 90th percentile is 8.46 x 10^{15} molecules/cm^2 and the TROPOMI 90th percentile is 5.58 x 10^{15} molecules/cm^2, with TEMPO aligning more closely (JSD of 0.133 compared to TROPOMI JSD of 0.265; Figure 3). TEMPO has 17.01% of data points above 7 x 10^{15} molecules/cm^2 for interstate values in July, whereas TROPOMI appears to underestimate the frequency of higher NO_2 levels more, with a cumulative frequency of 3.61% above that threshold. Near highways, TEMPO achieves a much better representation of the higher observed NO_2 with a 90th percentile of 9.34 x 10^{15} molecules/cm^2 compared to TROPOMI with a 90th percentile of 5.32 x 10^{15} molecules/cm^2. The JSD for TEMPO is 0.151 and TROPOMI is 0.201 for highway monitors, indicating that TEMPO has better alignment near highways. For non-roadway locations, both instruments show very good alignment (TEMPO JSD = 0.024; TROPOMI JSD = 0.023; Figure 3) with the monitor data distributions, with TEMPO and TROPOMI alignment with ground monitors being more comparable than in December 2023.

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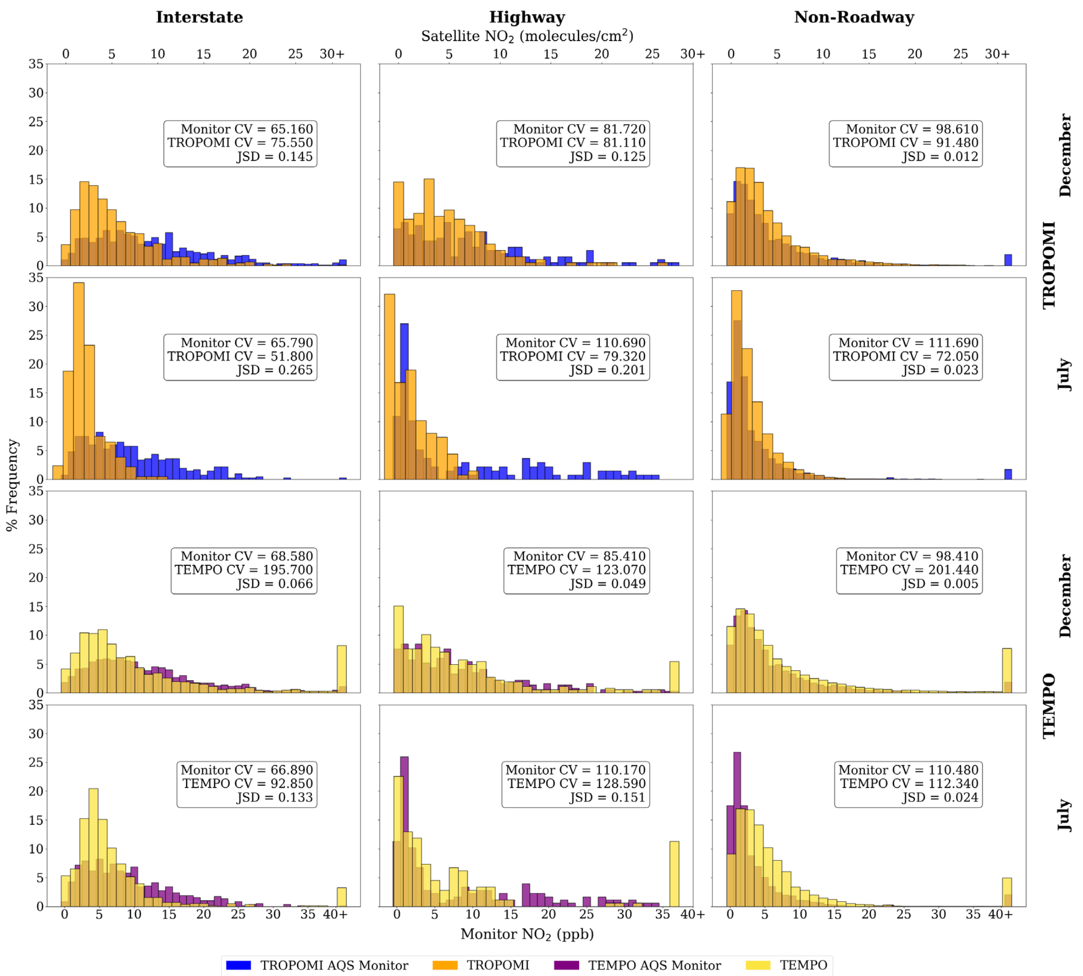

Figure 3. December 2023 and July 2024 frequency distributions of NO_2 as measured by AQS ground-based monitors filtered to the valid TROPOMI (blue) and TEMPO (purple), TROPOMI (light orange), and TEMPO (yellow) data for three monitor classifications: Interstate, Highway, and Non-roadway. The x-axes indicate the range of NO_2, with the primary, lower x-axis showing monitor NO_2 concentrations in parts per billion (ppb) and the secondary, upper x-axis showing TROPOMI NO_2 VCD and TEMPO NO_2 VCD in 10^{15} molecules per cm^2. The boxes show the Coefficient of Variation (CV) and Jensen Shannon Divergence (JSD) for each season and monitor classification.

Throughout both December 2023 and July 2024, TEMPO's improved alignment with ground-based monitors compared to TROPOMI may be attributed to several factors. TEMPO operates from a geostationary orbit, allowing it to take hourly measurements and capture the diurnal variability of NO_2 concentrations more effectively than TROPOMI, which has a single daily overpass time. This high temporal resolution enables TEMPO to better match the timing of NO_2 peaks and fluctuations detected by ground-based monitors, which are also recorded on an hourly basis. Additionally, TEMPO's finer spatial resolution, approximately 2 km in the north-south direction and 4.5 km in the east-west direction, may allow it to capture more localized pollution sources, such as traffic emissions along highways and interstates. This may be why we see such a large difference in alignment in the interstate and highway categories between TEMPO and TROPOMI, and very little difference in alignment in the non-road category. In contrast, TROPOMI's 4 km x 4 km (re-gridded) resolution and single overpass time may be less effective at capturing these localized variations. TEMPO's finer resolution in one direction and its frequent observations may enable it to more precisely match the spatial and temporal variability detected by ground-based monitors. The consistency of slight underestimation for both instruments in high-pollution areas like highways and interstates suggests challenges in fully capturing elevated NO_2 levels that occur near traffic sources. Overall, this indicates that while TEMPO generally provides a closer approximation of NO_2 distributions compared to TROPOMI, both satellite instruments show limitations, particularly in representing peak concentrations at high-polluting sites.

3.3 Column-Surface Diurnal Alignment

In this section we explore the hourly alignment among monitor observations and TEMPO observations. Figure 4 presents the hourly JSD for TEMPO NO_2 measurements compared with ground monitors categorized by interstate (red), highway (orange), and non-roadway (green) monitors for December 2023 (Figure 4a) and July 2024 (Figure 4b). The results highlight distinct diurnal patterns across road types and seasons, reflecting the influence of traffic emissions, atmospheric mixing, and insolation.

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In December 2023, all monitor categories exhibit similar trends in the early morning, with high JSD values (highway JSD = 0.358; interstate JSD = 0.331; non-road JSD = 0.210) indicative of moderate to poor alignment between TEMPO and ground-based monitors. This pattern, consistent with early morning rush hour emissions and limited atmospheric vertical mixing (Harkey and Holloway, 2024) as well as a decrease in TEMPO's measurement accuracy due to high solar zenith angles in the morning according to TEMPO documentation (NASA Langley Research Center, 2024), suggests that TEMPO may not capture rapid increases in NO_2 during high traffic and low mixing periods. By mid-morning, JSD has decreased for all road types (highway JSD = 0.085; interstate JSD = 0.067; non-road JSD = 0.027), indicative of good alignment, with non-road monitors showing the most significant improvement (87% increase in alignment). This pattern of better alignment in non-road monitor areas could be attributed to lower NO_2 levels away from major sources of emissions. As the day progresses in December, JSD values for highway and interstate monitors increase steadily (with highways fluctuating more) after 17 UTC (~12 pm LT), with highways increasing in JSD from 0.102 to 0.490 and interstates increasing from JSD 0.097 to 0.590, indicating worsening alignment in the afternoon and early evening. This pattern may reflect the re-accumulation of NO_2 due to afternoon traffic and the collapse of the boundary layer later in the afternoon (Harkey and Holloway, 2024), as well as the decrease in TEMPO's measurement accuracy in the evening (NASA Langley Research Center, 2024). Non-road monitors show less change in JSD through the day, suggesting that TEMPO alignment is more consistent in non-road monitor areas throughout the rest of the day, only fluctuating in JSD values between 0.009 and 0.05.

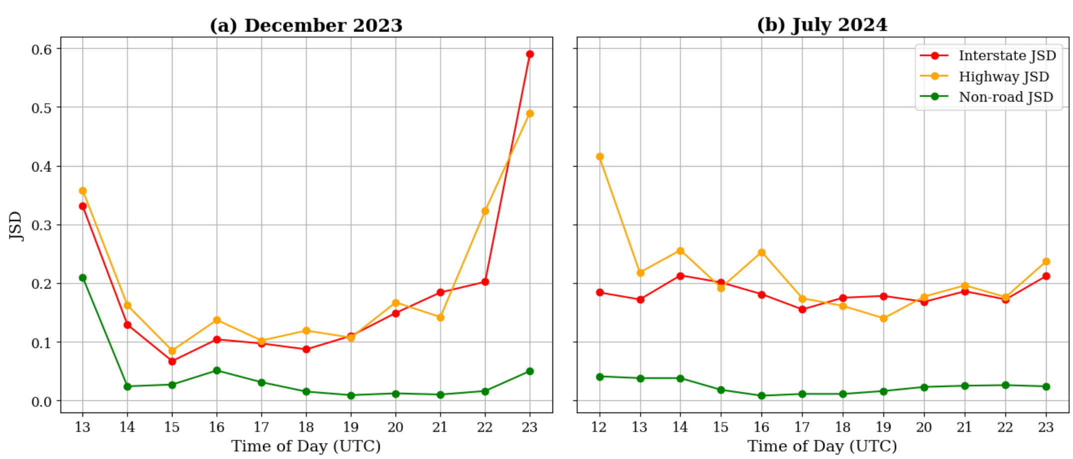

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Figure 4. The a) December 2023 and b) July 2024 hourly (UTC) TEMPO NO_2 Jensen-Shannon Divergences at interstate (red), highway (orange), and non-roadway (green) monitor locations.

In July 2024 highway and interstate monitors do not exhibit a clear diurnal pattern, with JSD values fluctuating between 0.14 and 0.416 for highways and 0.155 and 0.212 for interstates throughout the day. Consistent, localized traffic emissions and the shorter NO_2 lifetime during the summer suggest a less variable distribution of NO_2. Non-road monitors in July show somewhat worse alignment in the morning (JSD = 0.041), with improved agreement during the late morning and early afternoon (JSD ranging between 0.008 and 0.025). The non-road JSD remains fairly constant into the early evening, with alignment decreasing by about 13%, indicating that sunlight may play a larger role in the alignment in the evening since the sun is at a higher position in the sky during this time in the summer than in the winter (which increases in JSD at this time), enhancing TEMPO's measurement accuracy in the early evening in July.

Both months exhibit their highest JSDs, and worst alignment, in the early morning or early evening hours, which coincides with peak traffic times and the most uncertainty in TEMPO observations caused by the solar zenith angle. The best alignment and lowest JSDs occur sometime near midday (~10am LT to ~2pm LT).

The disparity between highways and interstates in TEMPO, where highways generally have the highest JSD, differs from the pattern seen with TROPOMI, where interstates tended to consistently exhibit worse alignment. This suggests that TEMPO's higher spatial and temporal resolution may capture localized sources more effectively, leading to variations in alignment based on the distribution and intensity of NO_2 sources.

4 Conclusions

This study evaluates the distributional alignment between satellite-derived NO_2 data from TROPOMI, TEMPO, and ground-based AQS monitors across the U.S. Our findings highlight several key points that inform the potential of satellite data for both regulatory and public health applications, particularly in informing future NO_2 monitor siting strategies.

The Jensen-Shannon Divergence (JSD) proved to be an essential tool in this study, offering a robust and interpretable metric for comparing the alignment and similarity of NO_2 distributions. Its symmetry and bounded range allowed us to evaluate the degree of similarity between satellite

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and monitor NO_2 values across different spatial and temporal scales, providing a clear quantitative framework for assessing the similarity of two different instruments.

In this study, we find a pattern of decreasing NO_2 with increasing distance from traffic sources, which is consistent with the findings of previous studies (Kimbrough et al., 2017; Karner et al., 2010; Richmond-Bryant et al., 2017). While ground-based monitors and TROPOMI satellite data may differ with proximity to roadways, particularly within 50-m, their measurements still follow the same overall trend. This convergence with increasing distance may be due to the reduction of localized near-road emissions and the broader atmospheric mixing captured more effectively by satellite observations at greater distances from roads. Using a larger buffer distance from roads (300 meters instead of 50 meters) improves the alignment between TROPOMI and monitor data, especially for highway monitor locations (JSD decreases by ~82%). The overall trend reflects the well-established gradient of declining NO_2 levels with increasing distance from traffic sources, and TROPOMI's ability to capture this trend, even if the specific values differ from AQS monitors in the near-road environment. Our findings indicate that TROPOMI tends to slightly underestimate surface NO_2 concentrations in areas with high traffic, such as interstates and highways, due to its spatial resolution and full-column measurements, which smooth out localized, ground-level pollution peaks captured by ground monitors. This is most evident in interstate monitors, where the JSD reveals the greatest divergence between satellite and monitor data (JSD = 0.158). These results are consistent with prior studies (Dressel et al., 2022; Kim et al., 2024; Ialongo et al., 2020), which also found that satellite instruments are less effective at capturing high NO_2 events near localized sources like traffic. The distributional alignment improves in non-roadway monitors (JSD = 0.009), where NO_2 levels are lower, and there are usually fewer localized sources of pollution. The lower pollution levels in these areas allow TROPOMI to more accurately reflect the conditions captured by ground-based monitors, leading to lower JSD values, and therefore better alignment. This trend suggests that TROPOMI may be particularly useful for monitoring air quality in rural or less polluted regions where ground monitors are sparse or absent.

Seasonality plays a critical role in the similarity of satellite and monitor data. Winter consistently shows the best alignment (JSD = 0.010), with the TROPOMI distribution capturing nearly the full gradient of NO_2 seen within the ground-based monitor distribution. This likely reflects the

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longer atmospheric lifetime of NO_2 in winter, which allows for better vertical mixing and less spatial variability (Harkey et al., 2015; Boersma et al., 2009; Shah et al., 2020). In contrast, summer shows the worst alignment (JSD = 0.035), which is likely due to the shorter lifetime of NO_2 and increased photochemical activity during warmer months, causing greater discrepancies between localized surface measurements and the satellite column. Similar conclusions were reached by previous studies (Shah et al., 2020; Karagkiozidis et al., 2023), indicating that seasonality is a crucial factor in assessing satellite performance for regulatory purposes. These seasonal differences underscore the need for considering temporal factors when evaluating the use of satellite data for monitor siting and NO_2 regulation.

The integration of TEMPO data into this study highlights its potential to advance our understanding of NO_2 distributions, especially when compared to TROPOMI. TEMPO's ability to provide hourly measurements at a finer spatial resolution offers significant advantages in capturing diurnal NO_2 patterns and detecting localized pollution events. Our findings from December 2023 and July 2024 demonstrate that TEMPO better captures the wide range of surface NO_2 measurements than TROPOMI, especially at higher NO_2 levels. TEMPO’s JSDs are almost always lower than TROPOMI’s, with JSDs ranging from 0.005 to 0.151 and TROPOMI’s JSDs ranging from 0.012 to 0.265. This improvement in alignment with ground monitors could be attributed to TEMPO’s better spatial and temporal resolution.

We also find that TEMPO is best at capturing ground-level NO_2 amounts around midday (~10am to ~2pm LT). This could be due to the lower traffic levels and therefore lower pollution levels during this time period, as well as a lower solar zenith angle, allowing TEMPO to have more accurate measurements. However, challenges remain in completely capturing high NO_2 levels during peak traffic times and accurately capturing NO_2 during high solar zenith angles in the morning and evening across monitor classifications. These results underscore the influence of spatial resolution, time of day, and measurement frequency on the ability of satellite instruments to align with ground-based NO_2 measurements. Future research should build upon these insights by incorporating longer time periods and multiple years of data as more TEMPO data becomes available to study long-term TEMPO distributions. The enhanced temporal and spatial resolution of TEMPO, alongside its comparison to other instruments like TROPOMI, provides valuable context for understanding the dynamics of NO_2 pollution, especially how it varies throughout the day, to improve strategies for air quality monitoring and public health protection.

This study offers insights for optimizing nitrogen dioxide monitor siting, enhancing regulatory planning, and supporting public health interventions. By demonstrating the strengths and limitations of satellite-derived NO_2 data, we highlight its potential to complement ground-based monitoring networks.

Code and Data Availability

All data used in this study are open to the public. Hourly NO_2 data from AQS were obtained from https://aqs.epa.gov/aqsweb/airdata/download_files.html. Copernicus Sentinel 5P Level 2 TROPOMI NO_2 data were processed by the ESA, Koninklijk Nederlands Meteorologisch Instituut (KNMI; https://doi.org/10.5270/S5P-s4ljg54), downloaded from the NASA Goddard Earth Sciences Data and Information Center (GES DISC) in January 2021, and gridded using WHIPS (https://sage.nelson.wisc.edu/data-and-models/wisconsin-horizontal-interpolation-program-for-satellites-whips/). TEMPO Level 3 NO_2 data were downloaded from NASA's EarthData Search (https://search.earthdata.nasa.gov/search/granules?p=C2930763263-LARC_CLOUD&pg[0][v]=f&tl=1732652660.361!3!!). Since all of our data is publicly available and the methods describe our calculations in detail, we did not make our code publicly available. The Jensen Shannon Divergence was calculated using the *scipy.spatial.distance.jensenshannon* python package.

Author Contribution

SA and TH conceptualized and designed methodology. MH helped with data curation. SA performed data analysis and visualization and prepared the original draft of the manuscript. All authors contributed to reviewing and editing the manuscript.

Competing Interests

The authors declare that they have no conflict of interest.

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