

Assessing Ozone Dynamics During the 2023 Summer STAQS Field Campaign Using Synergistic Observations and Model Simulations

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15 **Abstract.** NASA's Tropospheric Emissions: Monitoring of Pollution (TEMPO) geostationary satellite sensor provides high temporal and spatial resolution measurements critical for monitoring air quality. During the Synergistic TEMPO Air Quality Science (STAQS) component of the 2023 AGES+ campaign, extensive surface, airborne, and remote-sensing observations were collected over the New York City/Long Island Sound region, enabling comprehensive investigation of ozone and its precursors, including nitrogen dioxide (NO₂) and formaldehyde (HCHO). Evaluating TEMPO (version 3) NO₂ and HCHO
20 column retrievals against Pandora and GEO-CAPE Airborne Simulator (GCAS) observations, based on the limited number of coincident flight days available, shows TEMPO can capture urban-suburban pollution gradients and exhibits biases comparable to previous satellite validation studies with strong NO₂ column correlations ($R \approx 0.79 - 0.81$), though sharp transitions between high and low emission regions remain challenging. The high-resolution (1.33 km $\times$ 1.33 km) WRF-Chem simulation reproduces the major spatiotemporal patterns of surface ozone and NO₂ ($R \approx 0.56 - 0.73$), supporting its use to fill observational
25 gaps. Integrating TEMPO, WRF-Chem, in situ measurements, and ozone and wind lidar observations, we characterize the spatiotemporal ozone dynamics under different pollution regimes. High-pollution days involve early urban precursor accumulation and sea-breeze-driven coastal recirculation of pollutant-rich air. Moderate days exhibit localized enhancements driven by transport, such as downwind plume transport, while low-pollution days show efficient dispersion and limited ozone formation. This multi-platform framework highlights the importance of resolving fine-scale variability in coastal and transition
30 zones and illustrates TEMPO's potential for improving ozone forecasting and mitigation in complex environments.

1 Introduction

Poor air quality associated with elevated ozone (O_3) concentrations arises from transport and buildup of trace gas species such as nitrogen oxides (NO_x = nitric oxide and nitrogen dioxide: $NO + NO_2$), carbon monoxide (CO), and volatile organic compounds such as formaldehyde (HCHO), which photochemically oxidize to form tropospheric O_3 . These pollutants can negatively impact human health and Earth's natural ecosystems (U.S. EPA, 2020). At the surface, such gases are routinely monitored and regulated under the United States Environmental Protection Agency (EPA) National Ambient Air Quality Standards (NAAQS). Despite persistent mitigation efforts, the New York City/Long Island Sound (NYC/LIS) coastal region remains a frequent non-attainment area.

Coastal regions like NYC/LIS are complex due to the combination of dense urban emissions, proximity to large water bodies, and diverse meteorology. Emission sources in this environment are multi-faceted with heterogeneous biogenic and fossil fuel sources, shipping, and biomass burning emissions frequently transported from the western US and Canada (e.g., Wu et al., 2018; Gronoff et al., 2019; Yang et al., 2022; Ring et al., 2023; Su et al., 2025). Local meteorological processes, particularly sea and bay breezes driven by thermally induced mesoscale pressure differences, can recirculate pollutants between land and water and are frequently linked to inland O_3 exceedances (Miller et al., 2003; Banta et al., 2005; Darby et al., 2005; Loughner et al., 2014; Stauffer et al., 2015; Mazzuca et al., 2019; Li et al., 2020; Wang et al., 2023). These local-scale transport processes produce strong diurnal and spatial variability in pollutant concentrations (Tucker et al., 2010; Martins et al., 2012; Bernier et al., 2019).

Many modeling studies have highlighted the challenges of accurately simulating and forecasting coastal air pollution and meteorology due to sharp gradients in the planetary boundary layer (PBL) height, temperature, emission sources, and pollutant concentrations at the land-water interface, as well as the fine-scale structure of land/sea breeze circulations (Yerramilli et al., 2012; Dreessen et al., 2019; Sullivan et al., 2019; Zhao et al., 2020; Ma et al., 2021). These features often occur at finer spatial and temporal scales than conventional numerical models can resolve (Loughner et al., 2011; Goldberg et al., 2014). While high-resolution chemical transport models (CTMs) improve the representation of localized features on both the vertical structure and the temporal evolution of pollutants (Caicedo et al., 2019, 2021; Torres-Vazquez et al., 2022; Wang et al., 2023), they remain highly sensitive to input uncertainties and require robust observational constraints. Studies have demonstrated how O_3 can vary considerably across short distances, such as between the north to the south shores of Long Island (LI), as well as time-height variations due to differences in emission sources, meteorology, and deposition processes along coastlines (Mazzuca et al., 2017, Yang et al., 2022; Zhang et al., 2022; Tzortziou et al., 2023; Luo and Lu, 2024). Capturing these gradients and the mechanisms that drive them depends on sustained, high-resolution observations from ground-based, airborne, and satellite platforms to improve air quality modeling and forecasting.

Historically, in situ measurement networks have lacked the spatial and temporal resolution needed to resolve coastal local-scale pollution gradients, particularly over water (Zhang et al., 2020). This limitation has motivated numerous air quality field campaigns (<https://www-air.larc.nasa.gov/missions>), including DISCOVER-AQ, OWLETS, LISTOS, and TRACER-AQ,

to better understand coastal air quality processes. In 2023, NASA contributed to the multi-agency AGES+ campaign (AEROMMA+CUPiDS, ECAPE, STAQS and others) which encompassed several synergistic field efforts across U.S. urban regions. AGES+ collected comprehensive aircraft and ground-based measurements with extensive spatial and vertical coverage from July – August 2023. This study focuses on the STAQS campaign component which occurred in the NYC/LIS region and targeted the dynamic spatial and vertical structure of emissions and pollution over urban and coastal zones to study air quality and support early validation of the Tropospheric Emissions: Monitoring of Pollution (TEMPO) satellite.

The recent launch of NASA’s TEMPO geostationary satellite addresses current satellite observation limitations by providing hourly, high spatial resolution data products such as key O₃ precursors at $\sim 2.1 \times 4.4$ km² spatial resolution at the center of the field of regard (Chance et al., 2013; Zoogman et al., 2017). Using WRF-CMAQ and Pandora measurements, Tao et al. (2025) demonstrated the value of TEMPO hourly observations for investigating diurnal variability and surface–column relationships among HCHO, NO₂, and tropospheric O₃. Despite these advancements, satellite retrievals require validation, especially at urban/rural and land/water interfaces where retrievals can be challenging. During the STAQS field campaign, a suite of ground-based, airborne, and in situ instruments including Pandora, the GEO-CAPE Airborne Simulator (GCAS), ozonesondes, and multiple lidar systems were deployed to study spatiotemporal gradients and support satellite validation. In particular, lidars from the Tropospheric Ozone Lidar Network (TOLNet) have proven valuable for capturing large multi-dimensional O₃ variability driven by transport and emissions (Johnson et al., 2016; Gronoff et al., 2021; Bernier et al., 2022). Integrating these multi-platform observations with high-resolution models (e.g., CTM, backward trajectories) enables improved characterization of pollutant variability and source attribution, advancing satellite retrieval performance and surface air quality assessment in complex urban-coastal environments (Kotaskis et al., 2022; Phoenix et al., 2024).

In this work, we focus on the following questions: (1) How well does TEMPO capture the large spatiotemporal variability of O₃ precursors, NO₂ and HCHO, in a complex environment? To investigate this, we compare TEMPO retrievals to Pandora and GCAS measurements and consider both the spatial and temporal variability across the NYC/LIS region during the STAQS campaign. (2) What meteorological mechanisms and chemical conditions lead to the diverse pollution cases observed during this campaign period? To examine this, we conduct a high spatial resolution CTM simulation in conjunction with the campaign measurements to evaluate spatiotemporal patterns of meteorological and pollution conditions in the NYC/LIS region. Representative air quality cases are classified based on observed and modeled O₃ and meteorology to analyze atmospheric characteristics under different regimes (high, moderate, and low pollution). This framework also provides a basis for evaluating the conditions under which TEMPO more accurately captures precursor variability. All available datasets including model output, TEMPO satellite retrievals, ground-based and airborne in situ and remote-sensing observations, and TOLNet O₃ and Doppler wind lidar measurements are used to explore NO₂ and HCHO and their relationship to the multi-dimensional structure of O₃, and the chemical and meteorological drivers of pollution events. By combining modeling and multi-platform observations, this study provides a synergistic approach for characterizing atmospheric composition and O₃ dynamics as well as evaluating instrument performance in a complex coastal region.

2 Data and methods

2.1 TEMPO column NO₂ and HCHO retrievals

NASA's TEMPO satellite (launched April 7, 2023) measures atmospheric pollution from geostationary orbit in the UV+VIS wavelength range for the greater North America domain (Zoogman et al., 2017). The satellite makes a complete East to West scan of the field of regard every hour during daytime and provides high spatial resolution data ($\sim 2.1 \text{ km N/S} \times 4.4 \text{ km E/W}$ at 36.5°N , 100°W). For this project, we use TEMPO L2 version 3 (v3) NO₂ tropospheric and HCHO total column retrievals from August 2 to August 16, 2023. We oversampled the TEMPO satellite data using a physics-based approach from Sun et al. (2018) to match our custom model inner-most domain at $1.33 \text{ km} \times 1.33 \text{ km}$ resolution. TEMPO provides instantaneous retrievals, which were compared to the corresponding hourly model values. The TEMPO averaging kernels (AKs) were calculated following Eskes and Boersma, (2003) and Cooper et al. (2020) where W represents the scattering weight and AMF is the air mass factor:

$$\frac{W}{AMF} = AK \quad (1)$$

The AKs were applied to the model derived columns to account for measurement sensitivities and allow for a direct comparison with the TEMPO columns. For each day, we apply the recommended filters (quality flag and effective cloud fraction of < 0.2) to the L2 v3 vertical column density (VCD) data before calculating AKs and oversampling.

2.2 WRF-Chem configuration

To simulate air quality during the STAQS campaign we used the coupled meteorology-chemistry model, the regional Weather Research and Forecasting model with Chemistry (WRF-Chem; see Grell et al., 2005) model (version 4.2) on a nested domain over the NYC/LIS region for the duration of the campaign (July 26 – August 16, 2023) (Fig. S1). A summary of the key model configurations is displayed in Table S1 and described in more detail below. The spatial resolution of the outer, middle, and inner domains (D01, D02, and D03) are 12 km, 4 km, and 1.33 km. Model output is hourly and uses a total of 47 vertical levels from the surface to about 50 hPa.

The Model of Ozone and Related Chemical Tracers (MOZART4; Emmons et al., 2010) chemical mechanism coupled to the Global Ozone Chemistry Aerosol Radiation and Transport (GOCART; Chin et al., 2000) bulk aerosol approach mechanism was used along with the Tropospheric Ultraviolet and Visible (TUV) Radiation Model full photolysis scheme (Madronich, 1987; Tie et al., 2003), which applies climatological O₃ and O₂ columns. Other selected parameterizations include the Thompson microphysics scheme (Thompson et al., 2008), Rapid Radiative Transfer Model for General Circulation Models (RRTMG) longwave and shortwave radiation scheme (Iacono et al., 2008), revised MM5 Monin–Obukhov similarity scheme for surface layer modeling (Monin and Obukhov, 1954), NOAA Land-Surface Model (Niu et al., 2011), YSU boundary layer scheme (Hong, 2010), and Modified Tiedtke scheme for cumulus modeling (Zhang et al., 2011). The initial and boundary conditions for gas-phase species and aerosols for the outer domain (D01) are provided by the Whole Atmosphere Community Climate Model (WACCM; Gettelman et al., 2019) at $1^\circ \times 1^\circ$ and interpolated in space every six hours. For the meteorological

initial and boundary conditions, Global Forecast System (GFS) model outputs at 0.25° resolution are used for D01, while D02 and D03 receive boundary conditions from their respective WRF model outer domains.

For anthropogenic emissions, the United States Environmental Protection Agency (US EPA) National Emission Inventories (NEI) 2017 emissions dataset at $12\text{ km} \times 12\text{ km}$ resolution was used for D01. The D02 and D03 simulations are driven by the anthropogenic emission dataset Neighborhood Emission Mapping Operation (NEMO), which is produced at hourly intervals based on the US EPA NEI 2019 dataset, offset to the year 2023, and reprocessed to a spatial resolution of $1\text{ km} \times 1\text{ km}$ (Ma and Tong, 2022). Elevated point sources and shipping emissions are implemented from US EPA 2019 $12\text{ km} \times 12\text{ km}$ dataset for all three domains. Fire emissions are provided by the Fire Inventory from NCAR version 2.5 (FINN/2.5; Wiedinmyer and Emmons, 2022) and implemented along with biogenic emissions from the Model of Emission of Gases and Aerosols from Nature (MEGAN) with online calculations (Guenther et al., 2012). Lightning NO_x is calculated online and included in the MOZCART chemistry option using the Price and Rind, (1992) schemes with modifications based on Barth et al. (2012) and Wong et al. (2013). The simulation was performed with a 4-day spin-up applied. To ensure consistency in the comparison with TEMPO observations, we derived model-based tropospheric vertical column densities (VCDs) from WRF-Chem using TEMPO's tropopause pressure product and corresponding AKs.

2.3 Multi-platform measurements during the STAQS campaign

2.3.1 TOLNet O_3 vertical profiles

Established in 2012, TOLNet consists of seven O_3 lidar systems stationed across the United States and five mobile Small Mobile Ozone Lidar (SMOL) systems, that provide high vertical and temporal resolution measurements of O_3 mixing ratios (<https://tolnet.larc.nasa.gov>). For the last decade, many of these lidar systems have been deployed to participate in several air quality campaigns (e.g., DISCOVER-AQ, OWLETS, LISTOS, TRACER-AQ, AGES+) with measurements commonly used for model evaluation, satellite validation, and scientific investigation. The lidar systems apply Differential Absorption Lidar (DIAL)-derived retrieval algorithms as well as a central processing system. For the STAQS campaign region, four TOLNet lidars were deployed around the LIS with the goal of capturing unique spatiotemporal differences of O_3 along the urban/coastal interface (Fig. 1). The City College of New York (CCNY) Tropospheric Ozone Lidar System (NYTOLS) was located on the CCNY campus in the NYC urban region operating for 23 days during the campaign period. The NASA Goddard Space Flight Center (GSFC) TROPospheric OZone (TROPOZ) lidar was located on the southern shore of the LIS operating for 32 days. The Langley Mobile Lidar (LMOL; Berkoff et al., 2025) and NOAA Chemical Science Laboratory (CSL) Tunable Optical Profiler for Aerosol and oZone (TOPAZ; ASDC, 2025) lidars were both located on the northern coast of the LIS along the CT coast operating for 15 and 36 days, respectively. In this analysis, the high resolution lidar data is interpolated to match the coarser vertical levels and hourly output of the WRF-Chem model with the original high-resolution curtain figures included in the Supplementary Information (SI) (Fig. S16).

160 2.3.2 Pandora NO₂ and HCHO

Pandora remote sensing instruments, part of the Pandonia Global Network (PGN), are ground-based UV–VIS spectrometers that provide direct-sun column measurements of O₃, SO₂, NO₂, and HCHO at high temporal resolution (Herman et al., 2009). Slant columns retrieved using the spectral fitting algorithm from Cede et al. (2017) are converted to vertical columns using geometric AMFs. For this study, we used the Pandora NO₂ and HCHO VCDs from eight sites around the
165 NYC/LIS region from July 16 to August 16, 2023 (Fig. 1). Tropospheric NO₂ columns were derived by subtracting TEMPO-retrieved stratospheric columns from the Pandora total columns. All data is processed as part of the PGN (<https://www.pandonia-global-network.org/>, last access: 9 October 2024) and only data with a quality flag of 0 or 10 (high quality) were applied in this study. Pandora data were co-located to the nearest WRF-Chem model hour (± 30 minutes) and averaged to hourly means for comparison.

170 2.3.3 GCAS NO₂ and HCHO column measurements

The GCAS instrument provides high–spatial native resolution ($\sim 250 \text{ m} \times 250 \text{ m}$) airborne measurements of NO₂ and HCHO VCDs using the differential optical absorption spectroscopy (DOAS) technique, following the methodology described in Judd et al. (2019), across the 300–490 nm and 480–900 nm spectral ranges with a 0.6 and 2.8 nm spectral resolution (Kowalewski and Janz, 2014; Nowlan et al., 2018; Judd et al., 2020). During STAQS, GCAS was flown on the NASA DC-8
175 aircraft over the NYC/LIS region on July 26, 28 and August 5, 9, 2023, providing ~ 7 km swath width observations at a nominal altitude of 9 km. The GCAS NO₂ and HCHO VCD data was used in this study to validate TEMPO and analyze pollution spatiotemporal characteristics. To ensure comparability, the GCAS columns (below flight observations up to 9 km) were scaled to full tropospheric columns using scale factors derived from WRF-Chem vertical profiles of NO₂ and HCHO that account for the above-aircraft portion of the column. Only cloud-free scenes were included and GCAS observations were collocated within
180 30 minutes of the hourly TEMPO measurements, allowing direct comparison of coincident measurements across multiple flight passes.

2.3.4 Other airborne and ground-based measurement instruments and statistical methods

The NASA DC-8 aircraft instrument payload also included the Airborne Cavity Enhanced Spectrometer (ACES) measuring in situ NO₂. Doppler lidar data from the New York State (NYS) Mesonet sites
185 (<https://nysmesonet.org/networks/profiler>), as well as the autonomous Doppler lidar from NOAA CSL (<https://csl.noaa.gov/>) at the Yale Coastal Site, provided horizontal and vertical wind measurements. Ground in situ monitoring station datasets for meteorology and chemistry including the US EPA Air Quality System (AQS; <https://www.epa.gov/aqs>) surface network and the National Weather Service (NWS) Automated Surface Observing System (ASOS; <https://www.weather.gov/asos/>) providing observational surface O₃, NO₂, and wind speed and direction measurements (Fig. 1). The number of ground measuring sites
190 with continuous observations available vary by the parameter with 16 sites for O₃, 7 for NO₂, and 14 sites for winds.

The statistical metrics employed in this work are Pearson correlation coefficient (R), mean bias (MB), and root mean square error (RMSE). Since the wind direction is an angular variable (recorded in degrees), we calculate circular statistics for correlation coefficient and RMSE. For wind speed statistics when comparing to WRF, we filter out winds below 2 m s^{-1} as lower winds speeds tend to be variable in direction and bias the model results. To compare the in-situ observations and the simulated surface concentrations, we interpolate the nearest WRF-Chem simulation grid to the geolocations of the AQS and ASOS stations. For further analysis, we split our domain into three subregions: urban area (red symbols in Fig. 1), LI coastal (blue symbols in Fig. 1), and Connecticut (CT) coastal (green symbols in Fig. 1). The locations of the AQS and ASOS stations and the TOLNet lidar, Doppler lidar, and Pandora instruments used in this work are all indicated in Fig. 1.

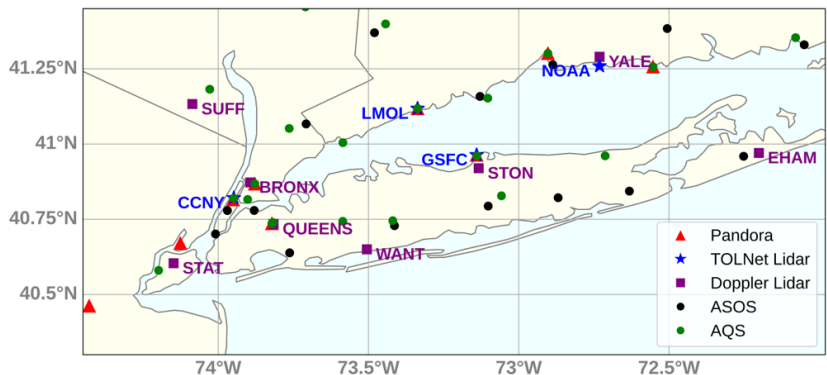


Figure 1: Map of the NYC/LIS study area covered during STAQS with subregions labeled: urban (red), LI coastal (blue), and Connecticut (CT) coastal (green) (full model domains shown in Fig. S1). Pandora stations, TOLNet lidar instruments, and ASOS/AQS monitoring sites denoted by discrete markers (marker legend displayed in the bottom right of the figure).

3 Results and discussion

In this section, we summarize key findings on O_3 and precursor species dynamics during the 2023 STAQS campaign and provide an initial assessment of TEMPO performance in a complex coastal environment. Sect. 3.1.1 compares high-resolution WRF-Chem simulations with ground-based observations, not as a detailed model evaluation but to demonstrate the model's utility as a tool to fill in measurement gaps. Sect. 3.1.2 evaluates TEMPO tropospheric NO_2 and total HCHO columns against Pandora and GCAS data to assess its ability to capture observed chemical conditions. Sect. 3.2 classifies the campaign period by O_3 level and meteorological regimes. Sect. 3.3 presents an integrated multi-platform analysis of pollution events, including high pollution days influenced by sea breeze circulation (3.3.1), moderate cases (3.3.2), and two contrasting moderate and low pollution days with a multi-platform perspective (3.3.3).

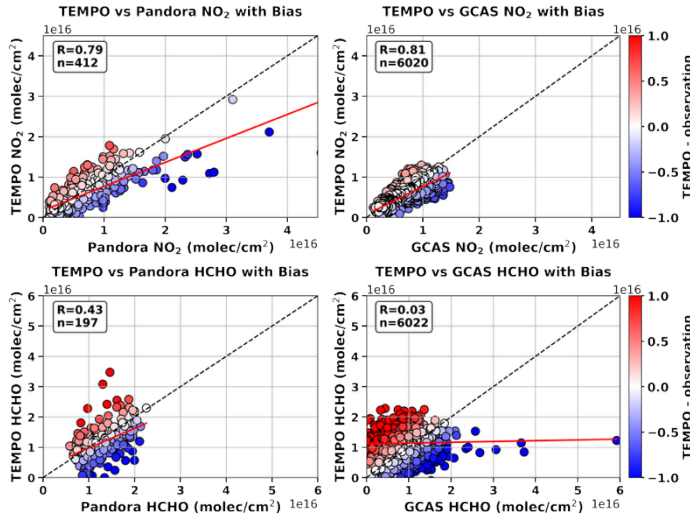
3.1 Model and satellite assessments

3.1.1 WRF-Chem O₃ and wind evaluation

WRF-Chem model simulations were evaluated at the finest resolution grid (1.33 km × 1.33 km) to determine its suitability as a tool for filling observational gaps during STAQS. Hourly AQS and ASOS observations of O₃, NO₂, wind speed, and direction were used for comparison (SI Fig. S2, Tables S2a). Overall, the model captures the spatiotemporal patterns of surface O₃ and NO₂ with moderate to strong correlations, reproducing key features. The diurnal time series comparison (Fig. S2) reveals a common model high O₃ bias overnight (Li and Rappenglueck, 2018; Travis and Jacob, 2019) and slight high bias during daytime O₃ peaks. Quantitative performance statistics computed across the full diurnal cycle indicate an overall slight overestimation of O₃ (MB = 4.4 ppb, NMB = 12.5%), and a more variable but slight underestimation of NO₂ (MB = -1.4 ppb, NMB = -19.1%).

To further investigate model performance across different regions of NYC/LIS, we subset the domain into three subregions: urban, LI coastal, and CT coastal (Table S2b). Results show the best performance for surface O₃ was in urban areas, with slightly lower correlations and higher biases along the LI and CT coasts. Model performance of surface NO₂ at all three locations is poor to moderate (R = 0.26 – 0.55) with the best performance in the urban region. Due to the importance of transport and sea breeze effect in coastal regions, we focus on the wind speed and direction parameters when evaluating the model simulated meteorological parameters. Surface level winds are simulated well overall, though urban wind speed and direction are more variable and slightly less accurate due to the calm and fluctuating conditions (R = 0.52 and 0.68, respectively). The coastal winds are better simulated with the highest correlations for wind speed and direction at LI coastal (R = 0.63 and 0.77, respectively) and CT coastal (R = 0.55 and 0.76, respectively) regions. In summary, WRF-Chem reproduces the main features of surface gaseous species and meteorology sufficiently to serve as a tool to fill observational gaps during the STAQS campaign.

3.1.2 TEMPO NO₂ and HCHO vertical column evaluation



235 **Figure 2: TEMPO comparison with Pandora (left column) and GCAS (right column) retrievals for NO₂ (top row) and HCHO (bottom row) (molec/cm²). Points are colored by the bias (TEMPO – Pandora or GCAS). The dashed black line indicates the 1:1 relationship and the solid red line shows the least-squares regression fit. Sample sizes are indicated in each panel (n).**

To determine the capability of TEMPO to observe complex pollution patterns in the NYC/LIS region, we investigate the agreement with independent instruments (Pandora and GCAS). We first investigate the overall statistical performance of TEMPO NO₂ and HCHO VCDs at Pandora sites (all campaign days) and along the entire GCAS flight paths (August 5 and 9, 2023) (Fig. 2). The results indicate that TEMPO has a strong correlation with both Pandora and GCAS ($R = 0.79$ and 0.81 , respectively) for NO₂ based on $n = 412$ and $n = 6020$ coincident matchups, respectively. Relative to Pandora, TEMPO performance varies with NO₂ magnitude, exhibiting a low bias at the highest VCDs measured by Pandora and improved agreement at lower VCD values. In comparison to GCAS, TEMPO NO₂ shows a slight low bias overall but less than compared to Pandora. For HCHO, TEMPO shows weaker correlation with Pandora ($R = 0.41$) and GCAS ($R = 0.02$) across the available coincidences. Biases indicate a more similar agreement between Pandora and TEMPO across both low and high HCHO VCD values. In contrast, comparison with GCAS reveal TEMPO has a negative bias at higher HCHO VCDs values as well as a strong positive bias at lower observed GCAS VCD values. The pronounced high HCHO VCD measurements captured by GCAS (Fig. 2) may be influenced by localized point or near-point sources sampled by the aircraft, resulting in sharp HCHO enhancements that are not fully captured by TEMPO. Similar localized HCHO plumes, associated with combustion processes and urban NMVOC emissions, have been reported in previous studies (Zheng et al., 2022; Zuo et al., 2023).

Site	NO ₂					HCHO				
	n	R	NMB (%)	RMSE (molec/cm ²)	Mean Pandora (molec/cm ²)	n	R	NMB (%)	RMSE (molec/cm ²)	Mean Pandora (molec/cm ²)
New Brunswick	44	0.80	-25.5	4.8e+15	5.6e+15	27	0.29	-1.6	6.2e+15	1.3e+16
Bayonne	52	0.65	-28.3	6.4e+15	1.4e+16	46	0.42	-8.4	5.1e+15	1.3e+16
Queens	49	0.75	-20.2	3.5e+15	1.0e+16	42	0.51	-13.3	5.5e+15	1.5e+16
Manhattan-CCNY	44	0.69	7.4	2.7e+15	7.4e+15	7	0.82	6.2	5.8e+15	1.3e+16
Bronx	49	0.72	11.1	2.4e+15	6.3e+15	--	--	--	--	--
Old Field	34	0.10	-7.6	1.2e+15	2.9e+15	--	--	--	--	--
Westport	51	0.25	62.0	1.7e+15	1.9e+15	34	0.24	-17.4	5.2e+15	1.3e+16
New Haven	46	0.31	-33.7	1.7e+15	3.8e+15	--	--	--	--	--
Madison	43	0.42	-1.2	9.9e+14	2.0e+15	41	0.14	-7.6	4.3e+15	1.0e+16

255 To gain further insight into localized patterns of TEMPO performance, we evaluate NO₂ and HCHO VCDs at each Pandora site for the campaign period (Table 1, Fig. S3). At urban sites (New Brunswick, Bayonne, Queens, Manhattan-CCNY, Bronx), TEMPO NO₂ agrees well with Pandora (R = 0.69 – 0.80), showing positive biases at Bronx and Manhattan-CCNY and negative biases at the remaining sites. At coastal sites (Old Field, Westport, New Haven, Madison), TEMPO shows mixed biases and lower correlations. This evaluation suggests TEMPO NO₂ columns capture the large contrast in NO₂ concentrations

260 between the urban core (Manhattan and Bronx) and surrounding transitional-suburban and transportation-influenced regions (Bayonne, Queens, New Brunswick). However, larger biases in these transitional (non-urban core) regions indicate that TEMPO does not fully resolve the steep NO₂ gradients at this urban-suburban interface and may exhibit elevated biases under lower background pollution conditions. TEMPO displays the poorest performance (largest biases) at the sites closest to the land-water interfaces (New Haven and Westport), suggesting possible retrieval complications and increased uncertainty at these

265 boundaries, likely driven by sharp surface albedo contrasts between land and water as well as differences between the true vertical distribution of NO₂ and the a priori profiles used. The diverse results based on site location have been highlighted for TROPOMI in Judd et al. (2020) and is attributed to the differences in spatial representativity between the satellite and Pandora instruments, especially in the case of sampling over a shorter time range such as a campaign study. Even though TEMPO is retrieving at a higher spatial resolution compared to TROPOMI, the subpixel variation in the area seems to still influence the

270 results when comparing with localized Pandora measurements and even more along complex interfaces. Overall, the TEMPO NO₂ performance relative to Pandora is reasonable, with biases falling within the range reported in other satellite validation studies where station-to-station performance can vary considerably (e.g., Ghahremanloo et al., 2025), including in challenging urban–suburban transition zones and complex coastal land–water boundary environments.

Pandora HCHO VCD measurements were unavailable at the Bronx, Old Field, and New Haven sites during STAQS.

275 At the remaining sites, correlations with TEMPO range from weak to strong, with small negative biases (-13.3 to -1.6%) at all

sites except for a positive bias at the Manhattan-CCNY station. Absolute errors are modest relative to column variability across both urban and coastal sites and can be attributed to many factors such as retrieval vertical sensitivity and a priori vertical profiles. Overall, the TEMPO HCHO relationship with Pandora aligns with previous studies using other satellite instruments, such as TROPOMI and GEMS, showing a general slight underestimation (Judd et al., 2020; Zhu et al., 2020; Kim et al., 2023).

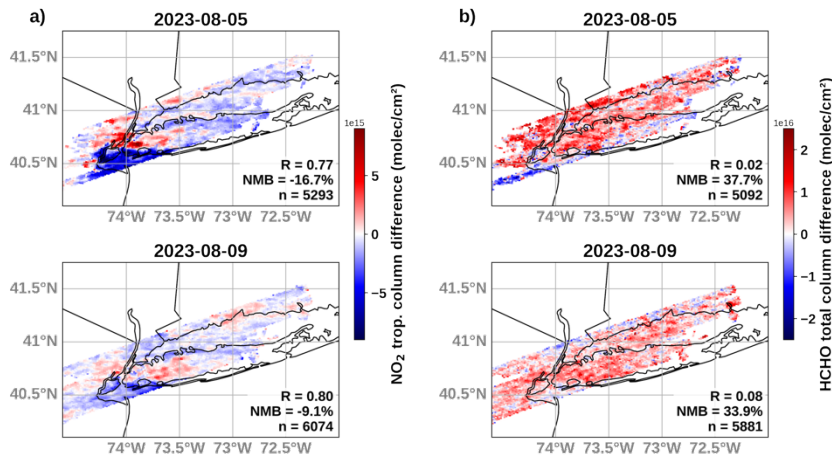
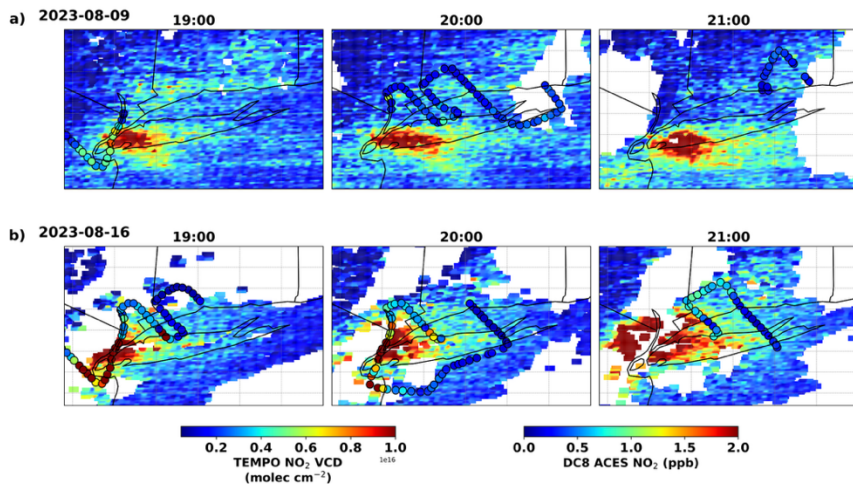


Figure 3: TEMPO - GCAS NO₂ (a) and HCHO (b) tropospheric VCD differences (molec/cm²) for two DC-8 flight days: August 5 and 9, 2023. The main statistics of these differences are displayed in the figure legend. Sample sizes are indicated in each panel (n).

Having established the overall TEMPO bias relative to GCAS, we next investigate how these differences vary across specific areas of the NYC/LIS domain by examining the full GCAS flight paths. Figure 3 provides a detailed view of the resulting NO₂ and HCHO differences (quantitative results in Fig. S4). On both days, TEMPO NO₂ exhibits a pronounced negative bias over Staten Island. This pattern may be partly attributed to the same albedo and reflectivity errors found with the near water Pandora sites, as well as the coarse spatial resolution of the a priori profiles used in the TEMPO retrievals. Conversely, directly over the NYC urban core, TEMPO NO₂ biases high with the bias stretching over the west end of LI. The bias differences from the core urban boroughs (Manhattan, Queens, and Brooklyn) to the more transitional urban-suburban Staten Island region are consistent with what was noted with the Pandora results. Although TEMPO captures the overall decrease in NO₂ across the urban-suburban/transitional boundary, the gradient is smoother than observed by GCAS. These results highlight the challenges of pixel-to-pixel retrievals of pollution variability, even with higher spatial resolution satellite retrievals. For HCHO, TEMPO retrievals exhibit weaker spatial correlations and moderate positive biases relative to GCAS, with noise dominating the signal. The differing HCHO bias behavior between TEMPO-Pandora and TEMPO-GCAS comparisons is consistent with previous studies showing that GCAS HCHO columns tend to be lower than Pandora (Rawat et al., 2025).

It is worth noting that HCHO validation studies typically rely on multi-day or monthly averaged retrievals to reduce retrieval noise and improve signal robustness (e.g., Johnson et al., 2023). The comparisons presented here use hourly TEMPO snapshots, which demonstrate TEMPO's unique geostationary capability but are inherently noisier and yield less statistically robust signals than those derived from longer temporal averages. The HCHO results should be interpreted as an illustration of

what is achievable with TEMPO's high-temporal-resolution observations under the sampling constraints of a campaign dataset, rather than as a comprehensive characterization of overall TEMPO HCHO retrieval performance. Caution is warranted when drawing broad conclusions from single-overpass comparisons of this nature.



305 **Figure 4: Hourly average TEMPO NO₂ VCDs (molec/cm²) overlaid with hourly ACES measured NO₂ (ppb) for the two DC-8 flight days: August 9 and 16, 2023.**

TEMPO tropospheric NO₂ VCDs were also compared with in situ NO₂ (ppb) measured by the ACES instrument aboard the DC-8 aircraft on August 9 and 16, 2023 (Fig. 4). While these products differ in units and vertical representation, the comparison serves as a qualitative illustration of spatial patterns and the connection between surface and column observations rather than a formal validation. On both days, ACES-measured NO₂ enhancements generally align with the elevated TEMPO tropospheric VCDs, particularly over the NYC urban core, suggesting well-mixed plumes and spatial consistency in the urban-suburban gradients in NO₂. Some mismatches occur such as along the LI coastline on August 16, 2023, where ACES captures sharp local gradients that are not as elevated in the TEMPO VCDs, likely reflecting the difference in vertical representation between the shallow in situ layer and the total column measurement. Overall, this qualitative agreement across multiple independent measurement types provides additional spatial context for interpreting TEMPO column retrievals. Combined with high-resolution WRF-Chem output, these observations allow us to bridge gaps among surface monitors, GCAS, and Pandora, providing a comprehensive view of O₃ dynamics and precursor species characteristics during the STAQS campaign.

3.2 Pollution regimes during STAQS

To investigate different characteristics of O₃ dynamics, we classify the STAQS campaign period into three O₃ pollution regimes: high, moderate, and low pollution. Classification is based primarily on observed peak hourly surface O₃ concentrations and the prevailing synoptic conditions, with thresholds informed by the distribution of O₃ levels across the campaign period rather than fixed regulatory standards. Based on observed and simulated surface O₃ concentrations, July 26 and 28, 2023 were classified as high pollution days; August 5, 6, 11, and 12, 2023 as moderate pollution days; and August 2

and 9, 2023 as low pollution days. These classifications are further supported in the following sections by the accompanying meteorological conditions from both in situ observations and model output, as well as the precursor species accumulation patterns from remote sensing observations.

The high pollution cases at the end of July occurred under a strong regional high-pressure system, with weak winds, high temperatures, and clear skies. The averaged observed surface winds for the high pollution regime (Fig. S5a) indicate winds were relatively weak and generally north-westerly to south-westerly ($225 - 315^\circ$). These stagnant conditions promoted photochemical buildup and local recirculation and transport of O_3 from the urban city to the coastal areas. Sea breeze circulation further enhanced coastal O_3 levels, with observed and simulated afternoon hourly exceedances (> 90 ppb) along the LIS coastlines. During the moderate pollution cases in early and mid-August, weaker synoptic forcing and transitional high-pressure systems produced light, variable winds and elevated temperatures. The averaged observed surface winds for these cases were much less consistent, which is typical under transitional synoptic conditions (Fig. S5b). These conditions brought moderate (~ 60 ppb) overall hourly O_3 levels but allowed for unique, localized O_3 formation. The low pollution cases on August 2 and 9, 2023, followed frontal passages that brought cooler temperatures, increased cloud cover, and scattered showers. Stronger synoptic winds, marine south-westerly winds on August 2, 2023, and continental northerly winds on August 9, 2023 (Fig. S5c) enhanced pollutant dispersion, resulting in low hourly average O_3 levels ($< 40 - 50$ ppb) across the region. Overall, these regimes capture the wide variability of hourly O_3 dynamics during STAQS, ranging from high-pressure dominate and sea breeze-driven exceedances to post-frontal events. These classifications provide the framework for the detailed multi-platform analysis in the following sections.

3.3 Integrated multi-platform analysis of pollution events

To comprehensively evaluate the mechanisms driving each pollution regime, model output was integrated with a range of surface, vertical profile, and column measurements. Surface data from WRF-Chem and AQS sites are used to establish general pollution behavior, while multi-dimensional profiles from TOLNet and Doppler lidars reveal regional transport, PBL mixing, and sea breeze circulations, with WRF-Chem providing spatial continuity where observational gaps exist. Satellite and airborne TEMPO and GCAS observations further capture the spatiotemporal evolution of precursor species, allowing for a thorough investigation of O_3 development during different pollution regimes.

3.3.1. High pollution and sea breeze cases (July 26 and 28, 2023)

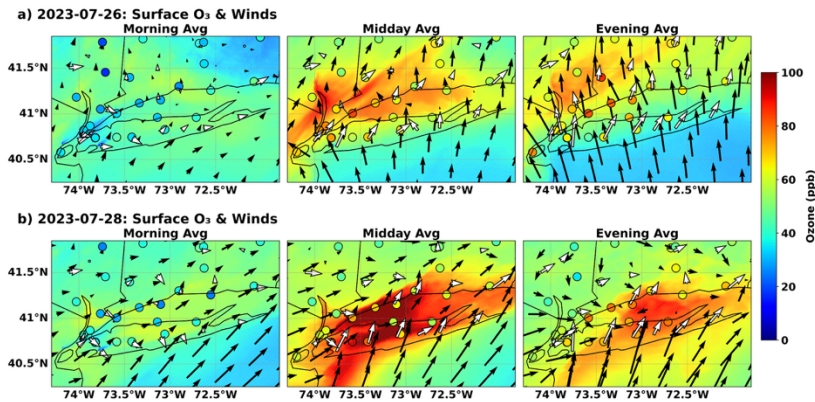
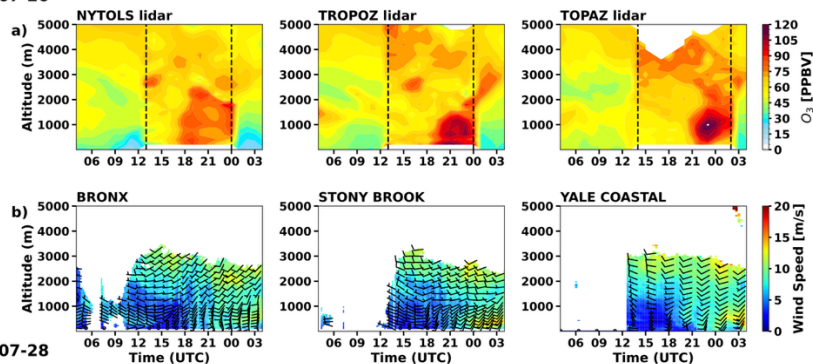


Figure 5: Morning, midday, and evening averaged AQS O₃ observations (scatter points) and ASOS winds (white arrows), overlaid with WRF-Chem simulated O₃ (contours) and winds (black arrows) for July 26 (a) and July 28, 2023 (b). Morning averages correspond to 11:00–15:00 UTC, midday to 15:00–19:00 UTC, and evening to 19:00–00:00 UTC.

The most prominent air pollution event occurred on July 26, 2023. Around midday, O₃ concentrations increased initially over the NYC urban core and western LIS before spreading eastward along both coastlines. The daily observed maximum O₃ (>100 ppb) peaked midday along the coast of the NY/CT border (Fig. 5a, Fig. S6a), driven by surface winds shifting from NW–W to S–SW in the afternoon. A classic strong sea breeze event involves the morning westerly transport of fresh urban emissions over the LIS, followed by a pronounced S–SE wind shift that recirculates the photochemically aged, O₃-rich air mass back inland toward NYC. The afternoon wind shift on this day (most notable at the LI coastal sites) is indicative of a sea breeze circulation; however, the transition is less sharp than in a classic strong sea breeze event where winds typically veer distinctly to S–SE (Fig. S7a). This more moderate sea breeze can still act to recirculate precursor-rich air masses inland, contributing to the observed O₃ buildup. While still resulting in elevated O₃ concentrations, the conditions on July 28, 2023, differed. Early/midday urban O₃ was on average much lower compared to July 26, 2023, while strong O₃ enhancements were observed on the southern LI coast (daily maximum O₃ > 90 ppb) and later building along the LI side of the LIS coastline before reaching the CT side (Fig. 5b, Fig. S6b). A similar NW–W to SW–S wind shift occurred, again consistent with a moderate sea breeze circulation rather than strong (most notable at the LI coastal sites) (Fig. S7b). Given the similar surface winds observed on both high pollution days (Fig. S7a, b), the differing O₃ accumulation patterns appear to be driven by other factors such as differences in emissions sources, PBL, and vertical mixing.

2023-07-26



2023-07-28

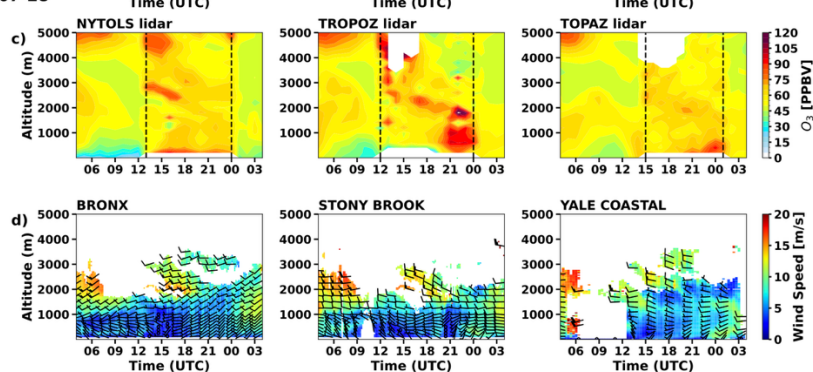


Figure 6: TOLNet lidar multidimensional O_3 (ppb) observations (outlined in black dotted lines) with WRF-Chem model simulated spatiotemporal O_3 filling missing data (a, c) and Doppler lidar (b, d) multidimensional wind profiles ($m\ s^{-1}$) observations at sites around NYC/LIS on July 26 and 28, 2023.

To provide additional perspective beyond surface observations, we also investigate the spatiotemporal distribution of O_3 and winds using the TOLNet O_3 and Doppler wind lidars (Fig. 6). The TOLNet lidars available on July 26, 2023, observed well-mixed high O_3 (~ 100 ppb) throughout the PBL (Fig. 6a) with the highest concentrations in the PBL indicative of a local O_3 formation. On this day, a clear progression of the pollution event was observed from its initiation at the NYTOLS lidar (urban core) which was then transported downwind over the LIS first to the TROPOZ lidar (LI side) and then finally to the TOPAZ lidar (CT side), corresponding with what was captured by the ground in situ network. The Doppler lidar vertical winds further demonstrate the sea breeze event captured by the surface ASOS monitors on this day (Fig. 6b). The observed wind shift is most notable at the urban location but is also apparent at the coastal locations. The urban wind shift extended up to ~ 1 km above the surface, indicating that the sea breeze circulation penetrated well into the mixed layer, recirculating urban emissions over the LIS and promoting a widespread increase of O_3 along both coastlines.

On July 28, 2023, urban in situ surface monitors measured relatively lower O_3 all day while the coastal sites observed elevated levels already by midday, suggesting that observed O_3 exceedances were not likely dominated by local photochemical production, in contrast to July 26, 2023. Often, O_3 exceedances can arise from the entrainment of pollutants from the previous day retained within the residual layer, which can be mixed into the growing PBL the following morning (e.g., Kaser et al., 2017; Sullivan et al., 2017). In other cases, these pollutants can be trapped overnight near coastlines and over the LIS under a

shallow marine boundary layer later getting mixed into the growing PBL and transported to nearby sites (Zhang et al., 2022; Torres-Vazquez et al., 2022). To assess whether these mechanisms may have contributed to the pollution events on July 28, we examined the simulated O₃ curtains as well as the observed wind lidar profiles spanning the overnight and early morning period (Fig. 6, S8). TOLNet observations on July 27 show elevated O₃ (75–105 ppb) persisting aloft at TROPOZ and TOPAZ through the late afternoon and into the evening (up to ~00 UTC July 28), providing observational evidence that an O₃ rich layer was present going into the overnight period (Fig. S8). Direct overnight observations are unavailable, however, WRF-Chem simulated O₃ curtains suggest elevated O₃ concentrations (60–75 ppb) may have persisted within the residual layer (approximately 1 – 2 km) through the overnight hours at these same sites. Consistent with this, the TOLNet observed profiles beginning near 12–13 UTC on July 28, 2023, capture elevated O₃ levels just above the surface layer that deepen vertically by mid-afternoon as the PBL develops (Fig. 6c), which is consistent with entrainment of residual layer air into the growing daytime PBL, though direct observational confirmation of the overnight transport itself is limited. There is also an overnight shallow marine boundary layer most notably present at the Yale Coastal site and slightly at the Stony Brook site (Fig. 6d), however, direct observational evidence of elevated O₃ within this layer is not available, and its contribution remains inferred from the surface timing and spatial pattern of the coastal enhancements. An alternative or complementary mechanism involves coastal convergence and recirculation within the LIS region, where interactions between the south-shore sea breeze and opposing coastal flows from Connecticut could favor O₃ accumulation; surface wind observations show some evidence of convergence along the northern LIS shore, though the signal is not strong enough to conclusively distinguish this from the residual layer entrainment pathway. These results are consistent with the early coastal O₃ enhancements on July 28, 2023, having been influenced by overnight pollutant accumulation in the residual layer and possibly shallow marine boundary layer, subsequently entrained into the daytime PBL during its initial growth that favored sustained coastal O₃ enhancements. However, given the reliance on model-simulated overnight structure and the plausibility of coastal convergence as a contributing factor, this interpretation should be regarded as a provisional hypothesis rather than a demonstrated mechanism.

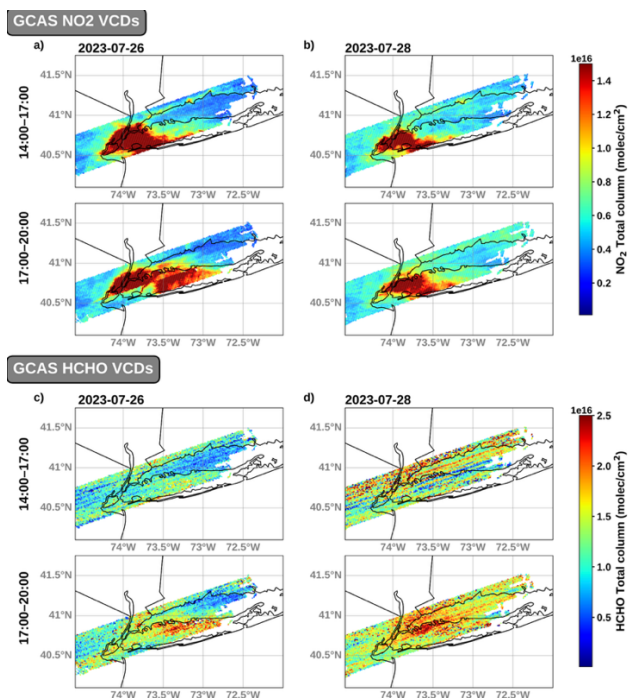


Figure 7: GCAS 3-hour averaged (14:00 – 17:00 UTC and 17:00 – 22:00 UTC) NO₂ and HCHO VCDs (molec/cm²) on July 26 and 28, 2023.

As TEMPO L2 data was not yet available in July 2023, GCAS measurements were used to investigate the O₃ precursor species development and potential O₃ sensitivity regimes during the high pollution cases (Fig. 7, Fig. S9). On July 26, 2023, GCAS columns confirmed a dense NO₂ plume over the urban NYC region during the late morning to early afternoon that aligns with the urban emission sources and corresponds to the highest NO₂ columns observed during the campaign (Fig. 7a). This early morning growth of pollutants is not surprising as the urban core usually provides fresh anthropogenic NO_x emissions, and the stagnant weather conditions were conducive to pollution accumulation. By late afternoon, high NO₂ was still observed over NYC and the majority of western and central LI (Fig. 7a). At the same time, GCAS captures some HCHO enhancements over the LIS and along both coastlines, suggesting possible enhanced VOC contributions to the O₃ photochemical production downwind/over water in a potentially more NO_x-limited region (VOC-rich) (Fig. 7c, Fig. S9a). This pattern is consistent with a fresh urban NO₂ plume undergoing photochemical processing as it is advected over the LIS and coincides with the transport event that led to the O₃ exceedances established with the surface and lidar measurements. On July 28, 2023, the morning NO₂ signal over the urban core is particularly weaker than July 26, 2023 (Fig. 7b). By mid-late afternoon, high HCHO / NO₂ column ratios (FNRs) dominate the LIS and coastal sites, coinciding with the high HCHO levels (Fig. S9b). Previous satellite studies over coastal regions, such as the Lake Michigan area, show that O₃ exceedance conditions are often associated with simultaneous increases in NO₂, HCHO, as well as the derived HCHO / NO₂ column ratio (Acdan et al., 2023). In this case, the temporal evolution is consistent with elevated HCHO and FNRs on July 28, 2023, broadly characterizing a VOC-rich environment later in the day, occurring after the initial coastal O₃ exceedances. This is consistent with the

entrainment-driven enhancement earlier in the day, followed by subsequent VOC-sensitive chemistry potentially contributing to the persistence of elevated coastal O₃.

The GCAS column measurements provide additional context for distinguishing two different types of coastal O₃ cases where a NO_x-dominated urban plume and sea breeze recirculation appear to have driven the July 26, 2023, event versus a more photochemically processed pollution regime on July 28, 2023, potentially influenced by residual pollution from prior days. FNR-based O₃ sensitivity inferences are qualitative given known uncertainties in HCHO retrievals; conclusions reflect broad photochemical regime characterization rather than a quantitative sensitivity diagnosis. Had TEMPO (or GCAS) data been available on the evening of July 27, 2023, the hourly columns could have provided more insight into the late-day buildup of O₃ aloft over the LIS, offering stronger evidence for the overnight residual layer and subsequent entrainment the next day. These high pollution cases represent two complex sea breeze events in which high spatiotemporal resolution measurements from TEMPO will be essential in future investigations providing valuable insight into the evolution and transport of pollution that might not be resolved with surface monitors.

3.3.2 Moderate pollution cases (August 5 – 6 and 11 – 12, 2023)

The conditions for the moderate pollution days resulted in unique, localized O₃ exceedances, defined here as brief hourly concentrations exceeding 70 ppb (not considered regulatory exceedances events based on the maximum 8-h O₃ average). Among the cases, August 6 and 12, 2023, exhibited similar O₃ patterns, so the remaining focus will be on August 11 and 12, 2023, where lidar and satellite observations provide deeper insight into transport and precursor species variability. The August 5, 2023, case is revisited in Sect. 3.3.1., while detailed analysis of O₃ and wind behavior on the August 5 and 6, 2023 cases are summarized in the SI (Text S1, Fig. S11, S12).

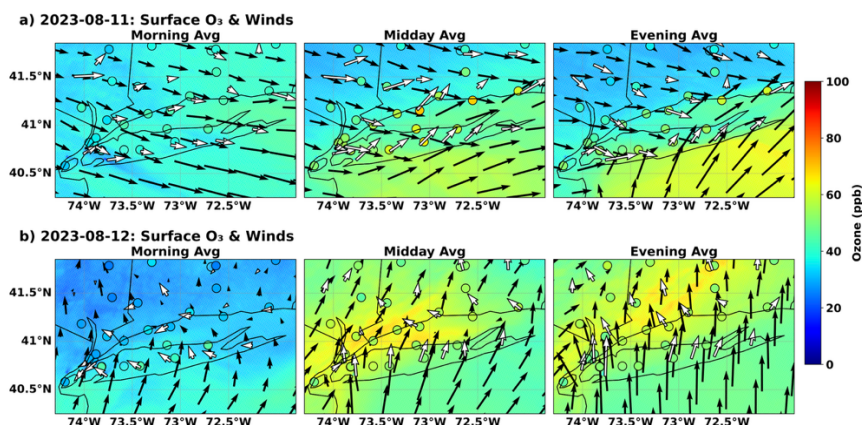


Figure 8: Morning, midday, and evening averaged AQS O₃ observations (scatter points) and ASOS winds (white arrows), overlaid with WRF-Chem simulated O₃ (contours) and winds (black arrows) for August 11 (a) and August 12, 2023 (b). Morning averages correspond to 11:00–15:00 UTC, midday to 15:00–19:00 UTC, and evening to 19:00–00:00 UTC.

On average, observed surface O₃ concentrations on August 11 and 12, 2023 were moderate but with a few localized hotspots (Fig. 8; Fig. S6e, f). On August 11, 2023, elevated O₃ (> 70 ppb) persisted in the afternoon for several hours in AQS observations along the CT coast, with steady W/SW winds (Fig. S7e) driving O₃ increases at the eastern end of the LIS. On August 12, 2023, surface O₃ reached a daily maximum (78 ppb) north of NYC shortly after peaking in the urban core of the city following a wind shift (E to S), with concurrent moderate levels of O₃ accumulating along the CT coast (Fig. S6f). Strong winds on this day transported polluted air far inland and north of the city (Fig. S7f), a pattern typical of downwind transport from major urban centers and often associated with localized hourly O₃ enhancements.

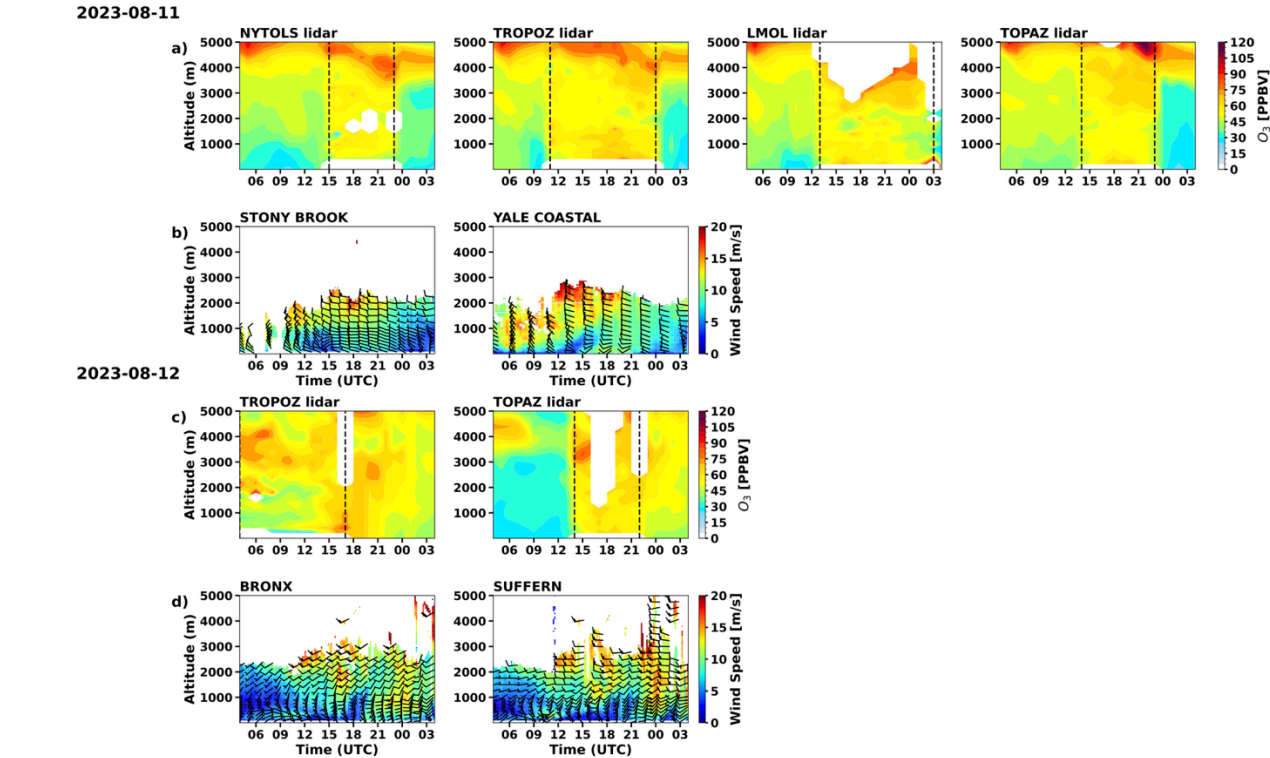


Figure 9: TOLNet lidar multidimensional O₃ (ppb) observations (outlined in black dotted lines) with WRF-Chem model simulated spatiotemporal O₃ filling missing data (a, c) and Doppler lidar (b, d) multidimensional wind profiles (m s⁻¹) observations at sites around NYC/LIS on August 11 and 12, 2023.

On August 11, the highest observed surface O₃ along the CT coast was captured first by the LMOL lidar and shortly thereafter by the TOPAZ system (Fig. 9a), consistent with the elevated O₃ measured at the nearby surface AQS sites. At the Yale Coastal site, Doppler lidar observations show weak westerly winds in the morning that strengthened and shifted slightly southwesterly by midday near the surface (Fig. 9b), a flow pattern consistent with alongshore transport and enhanced downwind influence along the CT coastline. This wind evolution coincides with the higher near-surface O₃ concentrations observed by the O₃ lidars located on the CT coast of the LIS (LMOL and TOPAZ). In contrast, winds at Stony Brook were more northwesterly, indicating that the site was influenced by a different air mass than the CT coastal sites, which likely limited

accumulations and is consistent with the relatively lower concentrations observed at that site. Consistently, the TROPOZ lidar at the same location detected elevated O_3 in the lower PBL that remained decoupled from the surface. Together, the co-located lidar observations on August 11, 2023, highlight the sharp mesoscale differences that can occur across the LIS where NY north shore experienced lower pollution and the CT coastline sustained hourly O_3 concentrations exceeding 70 ppb for multiple hours, though these do not constitute regulatory exceedances based on the MDA8 standard.

On August 12, 2023, moderate O_3 levels (~ 65 ppb) were observed along the CT coast by surface measurements and captured by the TOPAZ lidar (Fig. 9c). Near the urban region (Bronx), winds shifted from early morning easterlies to southerlies by evening, throughout ~ 1 km (Fig. 9d), while at Suffern, near-surface winds were stagnant, coinciding with the evening localized hourly O_3 enhancement (78 ppb) at the correspondent AQS site north of NYC. The CT coastline experienced easterly flow (Fig. 8b), resulting in a mesoscale convergence zone that contributed to the moderate O_3 along the CT coast. Near-surface O_3 evolution in downtown NYC could not be confirmed due to the unavailability of the NYTOLS lidar.

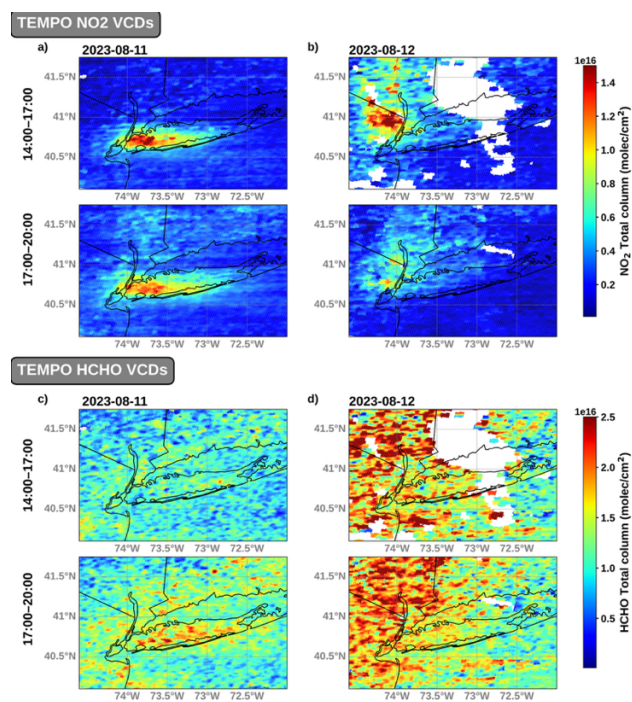


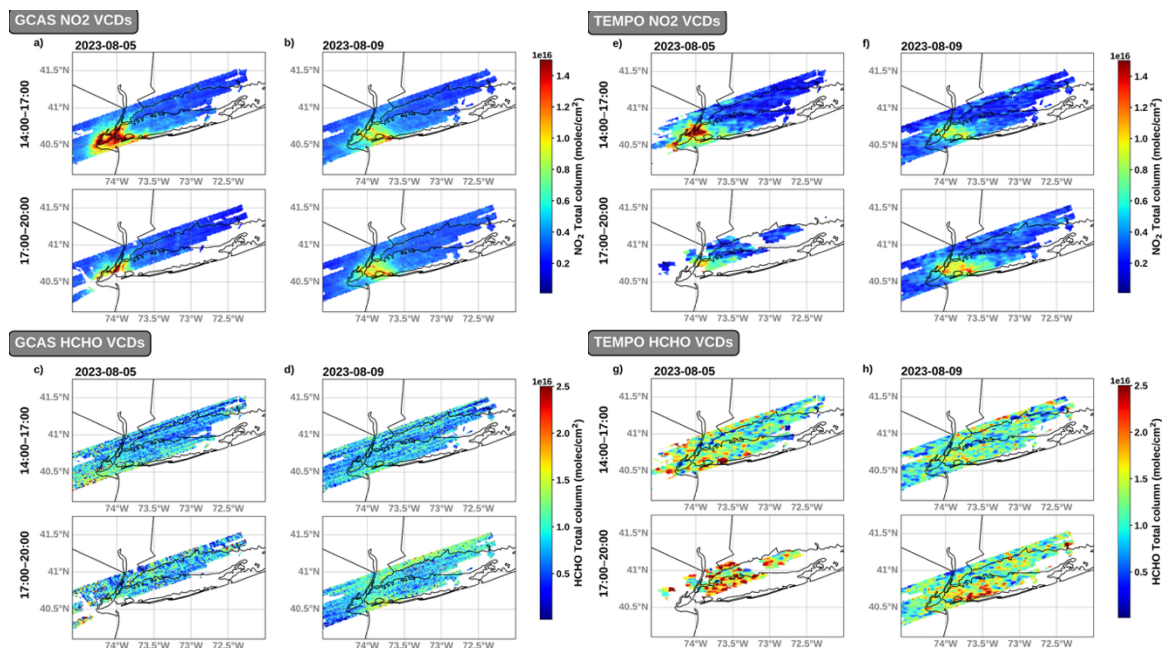
Figure 10: TEMPO 3-hour averaged (14:00 – 17:00 UTC and 17:00 – 22:00 UTC) NO_2 and HCHO VCDs (molec/cm²) on August 11 and 12, 2023.

TEMPO observations on August 11, 2023, show early-day NO_2 enhancements over the NYC urban areas and the southern LI coast, consistent with precursor accumulation in the source region (Fig. 10a). Later in the day, enhanced NO_2 persisted, followed by elevated HCHO over LI, suggesting possible photochemical processing and a potential transition toward a more VOC-rich chemical environment (Fig. S10a). The column measurements provide a spatially resolved picture of the precursor development and transport that complement the surface and lidar observations and help link upwind emission sources to the downwind O_3 response along the CT coastline that lasted many hours (Fig. 8a). The TEMPO observations on August 12,

2023, show similar patterns. High NO₂ was observed midday north of the NYC urban source region, urban region near the
 495 NJ/NY border, and west of the Hudson River. By the afternoon/evening, a slight NO₂ enhancement was observed just north of
 the CT coastline reaching the Yale Coastal location (TOPAZ lidar location). Higher HCHO is observed in the region in the
 morning hours (Fig. 10d) but NO₂ appears to dominate the chemical environment with a possible shift toward more VOC-rich
 conditions taking over by the evening hours (Fig. S10b). Given the known uncertainties in HCHO retrievals, these FNR-based
 regime inferences are treated as qualitative and spatially illustrative rather than as a definitive sensitivity diagnosis. The FNRs
 500 for these two moderate days nonetheless highlight the strong spatiotemporal variability of the chemical environment over the
 NYC/LIS region. These cases highlight the value TEMPO adds to interpreting the dynamics of pollution evolution, insight that
 cannot be captured by surface monitors alone. Future investigation of this variability using the hourly TEMPO observation will
 be particularly valuable to better resolve the evolution of precursor buildup and daily photochemical transitions.

3.3.3 Cross-comparison of moderate and low pollution cases (August 5 and 9, 2023)

505 With the additional moderate pollution and low pollution cases further summarized in the SI (Text S1, S2 and Fig.
 S11 – S14), the focus of this section is specifically on two moderate and low pollution representative cases – August 5
 (moderate) and August 9 (low), 2023, for which concurrent GCAS and TEMPO observations are available.



510 **Figure 11: NO₂ GCAS (a, b) and TEMPO (e, f) and HCHO GCAS (c, d) and TEMPO (g, h) 3-hour averaged (14:00 – 17:00 UTC and 17:00 – 22:00 UTC) VCDs (molec/cm²) on August 5 and 9, 2023.**

In comparison with the high and other moderate pollution cases in the previous sections (Fig. 7, Fig. 10), both GCAS and TEMPO notably indicate much lower NO₂ and HCHO enhancements near NYC and across the region on August 5 and 9, 2023 (Fig. 11). The notable higher dispersion of O₃ precursor species in these columns suggest that even if emissions were high

on this day, the meteorological and chemical conditions for these days did not allow for any major exceedances such as in the high pollution cases. This is particularly evident on the low pollution day, when strong winds associated with a cold front advected NO_x out of the source region, preventing elevated localized O₃ formation (Fig. 11b, d). For the moderate pollution case, there were two minor O₃ events: first the localized hourly enhancement on Staten Island and second the moderate increase along the CT coast. The NO₂ columns indicate high morning concentrations over Staten Island, Manhattan, and the western end of LI that are consistent with the emission buildup and upwind source of the O₃ enhancement later in the day. As established in the SI, the moderate O₃ increase along the CT coast was most likely not derived from the urban core source hence the low NO₂ signal in the column retrievals. Low HCHO columns on these two case days are consistent with minimal VOC-driven photochemistry and suppressed O₃ formation contrasting with the high and other moderate pollution days (Fig. 11e – h).

The availability of both GCAS and TEMPO on these two case days provides a multi-platform perspective on pollution and precursor variability under varying chemical and meteorological regimes. Generally, TEMPO and GCAS capture similar spatiotemporal patterns, though with some differences (Fig. 11). On the moderate pollution day, GCAS observed higher NO₂ over the urban core, particularly Staten Island and western LI, preceding the afternoon elevated O₃. TEMPO observed the same spatial pattern but with lower column magnitudes, consistent with Sect. 3.1.2. findings. Both TEMPO and GCAS FNRs suggest urban-to-suburban transitions, though given HCHO retrieval uncertainties these ratio-based patterns are treated as qualitative and spatially illustrative only, TEMPO shows a noisier spatial pattern due to HCHO retrieval noise and slightly higher ratios in regions where GCAS observes more NO_x-saturated regimes (Fig. S11). Overall, TEMPO appears to better capture both magnitude and temporal variability on the low pollution day, however, with only two flight days available, this result represents a preliminary inference and a more systematic evaluation across additional cases is needed before drawing broader conclusions about regime-dependent TEMPO retrieval performance.

4 Conclusion

NASA's TEMPO mission, with its unprecedented hourly geostationary observations of atmospheric composition over North America, offers new opportunities to investigate air quality from urban to regional scales. In coordination with the launch, the summer 2023 STAQS campaign delivered a set of airborne, surface, and ground-based measurements across the NYC/LIS region serving as a foundation for validating TEMPO trace gas retrievals (NO₂ and HCHO) and advancing the broader understanding of air quality in one of the most complex coastal urban environments in the United States. Leveraging these datasets, we evaluated TEMPO trace gas retrievals using Pandora and GCAS measurements across the NYC/LIS region. We employed a synergistic, multi-platform framework combining the in-situ measurements, ground-based and airborne remote sensing, and TEMPO v3 satellite retrievals during the campaign with a high-resolution (1.33 km × 1.33 km) WRF-Chem simulation. This approach allowed us to characterize regional pollution variability during the STAQS campaign period by capturing the evolution of O₃ and its precursors under a wide range of meteorological and chemical conditions.

The validation efforts during this study suggest TEMPO NO₂ column retrievals generally capture broad spatial patterns and magnitudes across the NYC/LIS region in comparison with Pandora and GCAS observations, with relatively best

performance over the urban core and reduced accuracy in urban–suburban transition and coastal zones. The limitations are due to multiple potential factors such as the steep gradients along transitional urban/suburban and coastal interfaces, low background concentrations outside of the urban region, surface albedo contrasts between land and water and reflectivity errors, and the a priori profile resolution, highlighting the importance of subgrid sensitivity even at high satellite resolution (Judd et al., 2020). TEMPO HCHO retrievals exhibit weaker correlations and moderate biases, reflecting the greater challenges associated with HCHO retrievals. Unlike validation studies that typically rely on multi-day or monthly averages to reduce retrieval noise, the HCHO comparisons here use hourly TEMPO snapshots; results should therefore be interpreted as an illustration of single-overpass retrieval behavior under campaign sampling conditions rather than a systematic characterization of HCHO retrieval performance. Despite these limitations, TEMPO shows capabilities in resolving spatial and temporal pollution gradients, consistent with recent studies demonstrating its value for near-surface air quality applications (Acker et al., 2025) and supporting improved O₃ forecasting and targeted mitigation in heterogeneous environments.

After establishing the performance of the TEMPO column retrievals and the high resolution model simulation, we used these products as tools alongside surface observations to identify and analyze three distinct pollution regimes during the campaign: 1) high pollution days, when stagnant summer conditions and early-morning precursor accumulation and sea breeze events which led to O₃ exceedances; (2) moderate pollution days, characterized by localized O₃ enhancements under transitional synoptic patterns; and (3) low pollution days, during which frontal passages enhanced dispersion and limited precursor buildup and O₃ formation. Integrating the TOLNet O₃ lidar and Doppler wind lidar profiles provided additional spatiotemporal context for these diverse chemical conditions, while TEMPO and GCAS observations enabled detailed examination of localized NO₂ and HCHO variability and its influence on O₃ chemistry across each pollution regime. The July high pollution cases illustrate how similar sea breeze patterns can produce very different O₃ outcomes depending on the vertical structure of pollutants and precursor availability. In the first case, the TOLNet O₃ and Doppler wind lidars and GCAS observations revealed a well-mixed BL and a deeper sea breeze circulation that recirculated a rich, late morning NO₂ plume from the NYC urban core over the LIS, producing strong downwind O₃ enhancements along both coastlines. In contrast, the second case showed minimal early NO₂ influences from the urban core. Instead, the lidar and GCAS observations, together with WRF-Chem simulated overnight structure, suggest that a more aged, O₃-rich residual layer plume may have persisted overnight and potentially contributed to elevated PBL and surface O₃ concentrations, however, direct overnight observations are unavailable and coastal convergence and recirculation represent a plausible alternative or complementary pathway. The moderate pollution cases in August highlighted sharp mesoscale differences within the NYC/LIS region, consistent with previous studies (e.g., Zhang et al., 2022; Tzortziou et al., 2023). Lidar and TEMPO observations are consistent with upwind NO₂ emissions and HCHO production contributing to downwind O₃ responses along the CT coast and north of NYC. Low pollution cases in August highlight how meteorology regulates precursor concentrations controlling the photochemical O₃ production on these case days. Cross-comparison of multi-platform observations (TEMPO and GCAS) allowed us to evaluate TEMPO retrieval performance under moderate and low pollution regimes. Based on the available two-day GCAS dataset, TEMPO appears to better capture O₃ precursor species variability under cleaner conditions, while at the urban-suburban transition zones in the more complex

moderate pollution case the performance appears more limited; however, this represents a preliminary inference from a limited sample and should be confirmed with more extensive observations.

Overall, the TEMPO and GCAS measurements used in this analysis provide new insight into complex coastal O₃ precursor species dynamics and demonstrate the value of integrating satellite, airborne, and surface observations to diagnose pollution evolution in heterogeneous environments. A key limitation of this study pertains to the sparse availability of many instrument's datasets included in the analysis. Pandora and GCAS retrievals, while essential to validation, have their own uncertainties and biases independent of the intercomparison with TEMPO. Furthermore, the observations have limited spatiotemporal coverage resulting in minimal numbers of coincident points between TEMPO and GCAS/PANDORA which may introduce a sampling bias. GCAS only flew for two specific days during the STAQS campaign and Pandora data have limited spatial coverage. The synergistic multi-platform framework requires temporal and spatial averaging which is necessary to achieve consistency across datasets but for shorter lived species such as NO₂, this approach may smooth sharp gradients and introduce additional uncertainty in column comparisons. Despite these constraints, the consistency in spatial patterns, column to surface relationships, and regime-dependent precursor variability across the datasets lends confidence to the robustness of the identified pollution cases. Beyond validation, these results advance the understanding of how O₃ pollution evolves in a multifaceted urban-coastal environment under different meteorological and chemical conditions. This analysis suggests that similar mesoscale transport mechanisms can result in distinct surface O₃ cases depending on recirculation, the vertical distribution of pollutants, and chemically favorable conditions, underscoring the critical role of a multi-dimensional perspective in regulating localized hourly O₃ enhancements. The regime-based framework further emphasizes how TEMPO performance may be dependent on atmospheric conditions and how this context should be considered when interpreting geostationary observations. Together, these findings highlight the value of geostationary sensors, and in this case unique high-spatiotemporal column measurements, alongside high-resolution in situ and remote sensing observations for resolving multi-dimensional pollution structure and improving our understanding of photochemical evolution and pollutant transport beyond what surface monitoring networks alone can capture, particularly within a chemically evolving complex coastal environment (Tao et al., 2022). Future work will benefit from the evaluation of updated TEMPO retrieval versions, including improvements in surface albedo treatment, and from further assessment of TEMPO O₃ profile retrievals across sharp urban-coastal gradients to refine interpretation of O₃ vertical structure and its relationship with surface pollution and mitigate O₃ episodes.

Code, data, or code and data availability

Python scripts used to reprocess TEMPO data, generate composites of TEMPO data as well as the reprocessed TEMPO composite data files we created in netCDF format are available upon request (send correspondence to Claudia M. Bernier: claudia.m.bernier@nasa.gov). TEMPO NO₂ and HCHO data were downloaded from the NASA Goddard Earth Sciences Data website: <https://search.earthdata.nasa.gov> (last access: 4 November 2024). The reprocessed TEMPO NO₂ and HCHO data can be downloaded from <https://websiteswithdata>. Ground-based AQS surface O₃ and NO₂ monitor data can be downloaded from

the U.S. EPA Air Data website: <https://www.epa.gov/outdoor-air-quality-data> (U.S. EPA, 2022). Ground-based ASOS surface wind monitor data can be downloaded from the NCEI NOAA Integrated Surface Dataset website: <https://www.ncei.noaa.gov/access/search/data-search/global-hourly>. Pandora monitor data can be downloaded from the Pandonia Global Network website: <https://data.hetzner.pandonia-global-network.org> (last access: 9 October 2024). TOLNet data were downloaded from <https://tolnet.larc.nasa.gov/download> (last access: 30 August 2024). Wind doppler lidar data were downloaded from the New York State (NYS) Mesonet sites <https://nysmesonet.org/networks/profiler> (last access: 5 June 2025)., as well as from NOAA CSL website <https://csl.noaa.gov/> (last access: 5 June 2025).

620 **Supplement link**

The link to the supplement will be included by Copernicus, if applicable.

Author contributions

CMB and MSJ designed the experiments, and CMB carried them out. CMB developed the model code and performed the simulations and evaluations. CMB prepared the manuscript with contributions from all co-authors. JS, GG, FM, and RA
625 provided the processed TOLNet O₃ lidar datasets. LJ provided the processed GCAS datasets.

Competing interests

The contact author has declared that none of the authors has any competing interests.

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Review statement

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