



Supplement of

Assessing ozone dynamics during the 2023 summer STAQS field campaign using synergistic observations and model simulations

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1 **S1. Moderate pollution cases (August 5 – 6, 2023)**

2 On August 5, 2023, average surface O₃ concentrations were moderate, with the maximum value (76 ppb) observed
3 near Staten Island (Fig. S12a, Fig. S6c). Winds on this day were generally low and displayed large spatial and directional
4 variability (Fig. S7c). The stagnant conditions on this day inhibited the transport of pollutants outside of the urban region
5 which delineates the location of the O₃ exceedance. In the afternoon of August 6, 2023, the maximum O₃ concentration (77
6 ppb) was observed in downtown NYC, followed by an exceedance (76 ppb) just north of downtown (Fig. S12b, Fig. S6d).
7 This localized event is supported by the observed surface winds in the region shifting (from E/NE to S/SE) acting to transport
8 the NYC polluted air mass downwind (Fig. S7d).

9 On August 5 and 6, 2023, the TOLNet lidars observed less vertically mixed PBLs (Fig. S13a, c), with all lidars
10 observing a well-defined elevated O₃ plume above 3000 m a.g.l. that does not necessarily or always coincide with higher O₃
11 in the PBL or at the surface. On August 5, 2023, there were two different local build-ups in the region, one exceedance on
12 Staten Island and then some moderate O₃ accumulation along the CT coastline (Fig. S13a, Fig. S6c). The O₃ lidar in the NYC
13 urban region (NYTOLS) never measured levels above 45 ppb near the surface and the elevated O₃ (70 ppb) captured by the
14 lidar on the LI coast (TROPOZ) does not reach the surface. The only lidar that measured elevated near surface O₃ is the location
15 near Yale Coastal along the CT coast (TOPAZ), corroborating the surface monitoring sites. With light, variable winds coming
16 from the NW – NE urban region (Fig. S7c), the localized build-up captured by the surface monitors near Staten Island can be
17 explained as a downwind transport case. On the other hand, the moderate accumulation along the CT coastline does not seem
18 to be locally transported pollutants from the urban core. Strong winds at Yale Coastal (~ 10 m/s), near the O₃ build up at the
19 CT coast, persisting all day throughout the first 5000 m a.g.l., is characteristic of a synoptic-scale transport regime rather than
20 a locally transported or recirculation (sea breeze) event. The continental air mass being advected at the CT coast could be well-
21 mixed background O₃. These two localized O₃ events (Staten Island and CT coast) on the same day both resulted from transport,
22 but at different scales: mesoscale downwind of urban plume and regional-synoptic long-range transport. The conditions on
23 August 6, 2023, are very similar to August 12, 2023, downwind urban core case that led to a north NYC exceedance. In this
24 case, the winds near the surface are not as strong in the afternoon (Fig. S7d, Fig. S13d). This put the O₃ build-up north of the
25 city but not as downwind nor as elevated as the other moderate case.

26 **S2. Low pollution cases (August 2 and 9, 2023)**

27 On average, observed O₃ was low on both August 2 and 9, 2023, with daily maximum only reaching 57 ppb and 49
28 ppb, respectively (Fig. S14a, b, Fig. S6g, h). August 2, 2023, was characterized by low, variable winds shifting from early
29 morning continental to southerly evening winds (Fig. S7g). August 9, 2023, had strong, consistent continental winds (Fig.
30 S7h). There were no notable near-surface pollution build-ups observed by the four TOLNet lidars on either day (Fig. S15) with

31 generally consistent directional winds observed throughout the BL on both days. These immediate post-frontal days were
32 transport effective for pollutant dispersion leading to low pollution conditions.

Table S1. Key configurations for the WRF-Chem v4.2 simulation

Model configurations	
Anthropogenic	NEMO based on the US EPA NEI 2019 (1 km)
Horizontal	nested domains: 12, 4, 1.33 km
Vertical	47 levels; surface - 50 hPa
Initial/boundary	Meteorology: GFS (0.25°), Chemical: WACCM (1° x 1°)
Chemistry	Gas scheme: MOZART-T1, Aerosol scheme: GOCART
Other emissions	Fire: FINNV2.5, Biogenic: MEGAN,
Parameterizations	Thompson, Modified Tiedtke, RRTMG, YSU, revised Monin-Obukhov, Noah, full TUV, Lightning-NOx

Table S2. Mean surface statistics model versus observations

a) full domain					
	n	R	MB (ppb)	NMB (%)	RMSE (ppb)
O ₃	528	0.74	5.1	14.7	10.7
NO ₂	527	0.56	-2.2	-28.0	4.3
	n	R	MB (m/s, °)	NMB (%)	RMSE (m/s, °)
wind speed	528	0.68	0.7	27.0	1.4
wind direction	528	0.73	-5.2	4.7	57.8
b) sub regions					
	n	R	MB (ppb)	NMB (%)	RMSE (ppb)
O ₃					
urban	528	0.75	2.4	7.0	9.8
LI coastal	528	0.63	3.5	9.2	12.0
CT coastal	528	0.70	4.8	13.0	12.6
NO ₂					
urban	505	0.55	-0.2	-2.4	5.3
LI coastal	503	0.39	-0.6	-27.5	1.6
CT coastal	506	0.26	-4.2	-62.8	6.4
	n	R	MB (m/s, °)	NMB (%)	RMSE (m/s, °)
wind speed					
urban	528	0.52	0.5	13.4	1.8
LI coastal	528	0.63	0.9	31.9	1.8
CT coastal	528	0.55	0.9	35.5	1.8
wind direction					
urban	395	0.68	-4.1	-1.1	65.5°
LI coastal	340	0.77	-5.7	-1.6	54.1°
CT coastal	325	0.76	0.2	0.0	56.1°

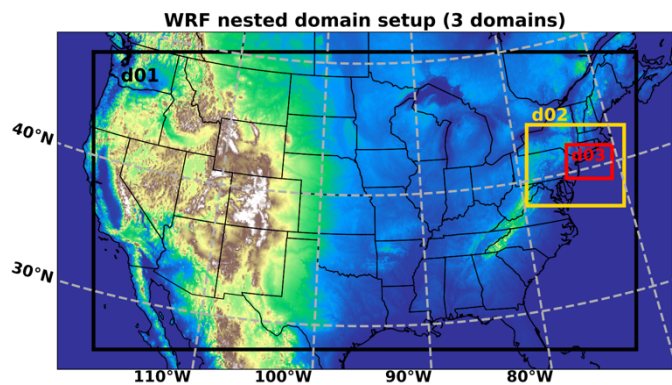


Figure S1: WRF-Chem model domain configuration: 12 km $\times$ 12 km (D01), 4 km $\times$ 4 km (D02), and 1.33 km $\times$ 1.33 km (D03) spatial resolutions.

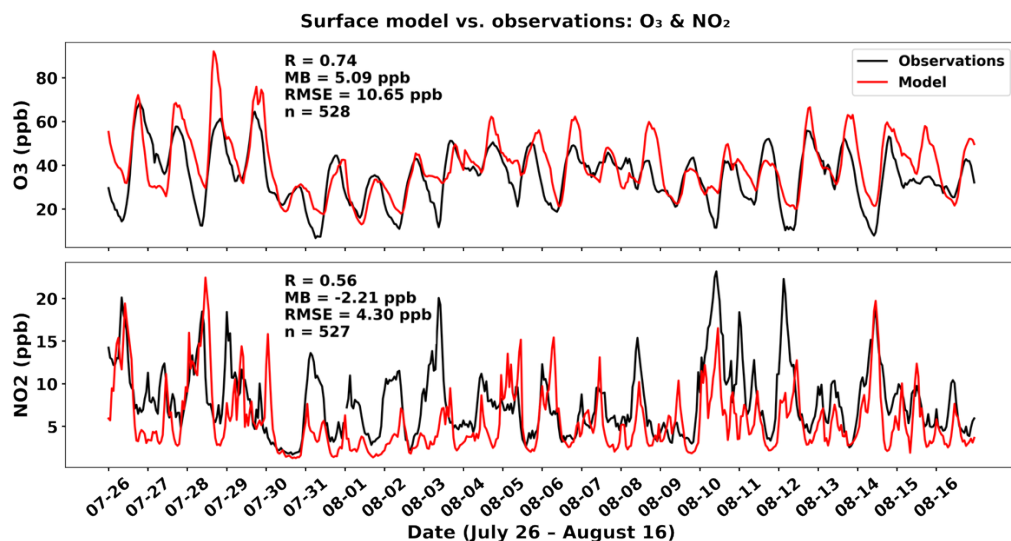
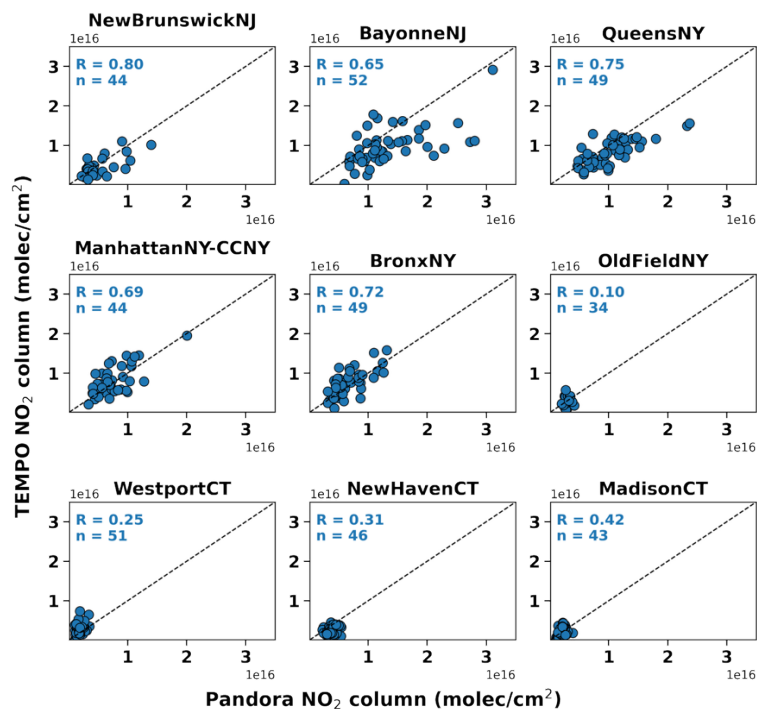


Figure S2: Hourly-averaged observed (black) and simulated (red) surface O₃ and NO₂ (ppb) timeseries during the STAQS campaign period (July 26 – August 16, 2023). The statistical comparison (correlation (R), mean bias (MB), and root mean squared error (RMSE) of the model and surface observations are provided in the inset of the figure. Sample sizes are indicated in each panel (n).

NO₂ Pandora vs TEMPO: correlations by site



HCHO Pandora vs TEMPO: correlations by site

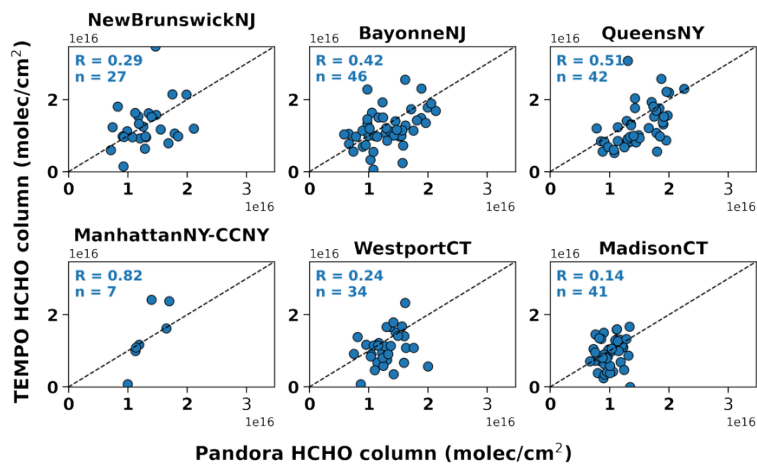


Figure S3: TEMPO vs. Pandora VCD comparison at each Pandora site in the NYC/LIS region for NO₂ (a) and HCHO (b) (molec/cm²). The correlation of TEMPO and Pandora observations are provided in the insets of each panel. Sample sizes are indicated in each panel (n).

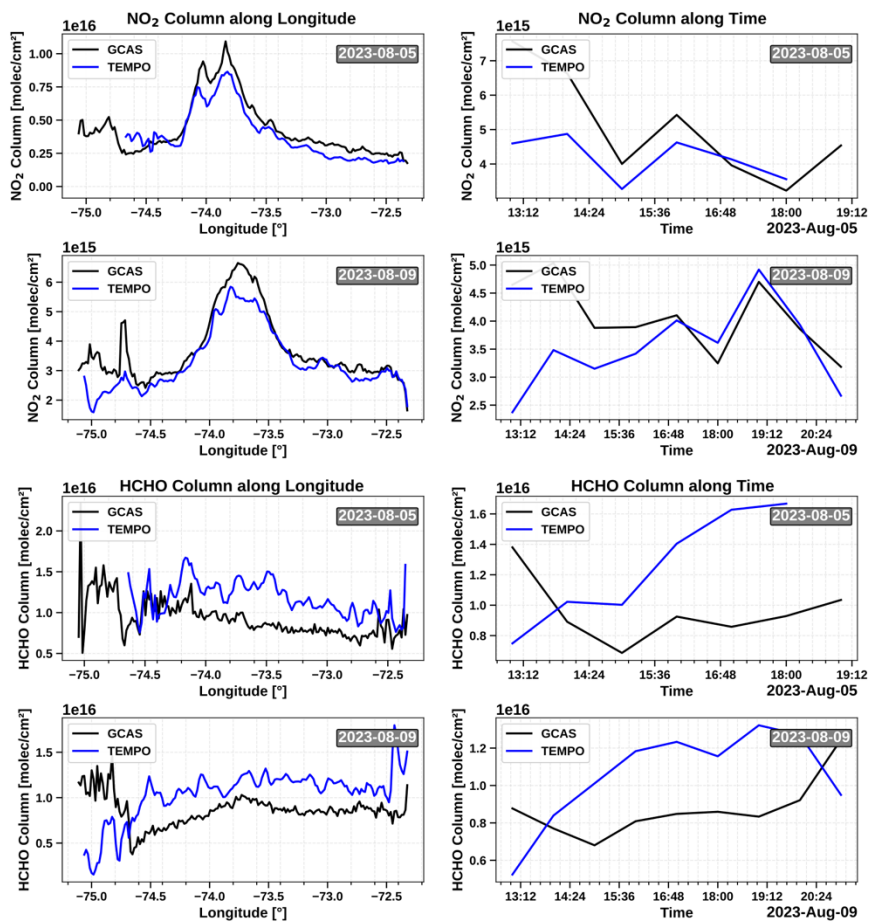


Figure S4: Comparison of NO₂ and HCHO VCDs (molec/cm²) averaged over longitude (left column) and time (right column) for August 5 and 9, 2023 from GCAS (blue) and TEMPO (black). Note that the y-axis values for NO₂ and HCHO are not consistent between figure panels.

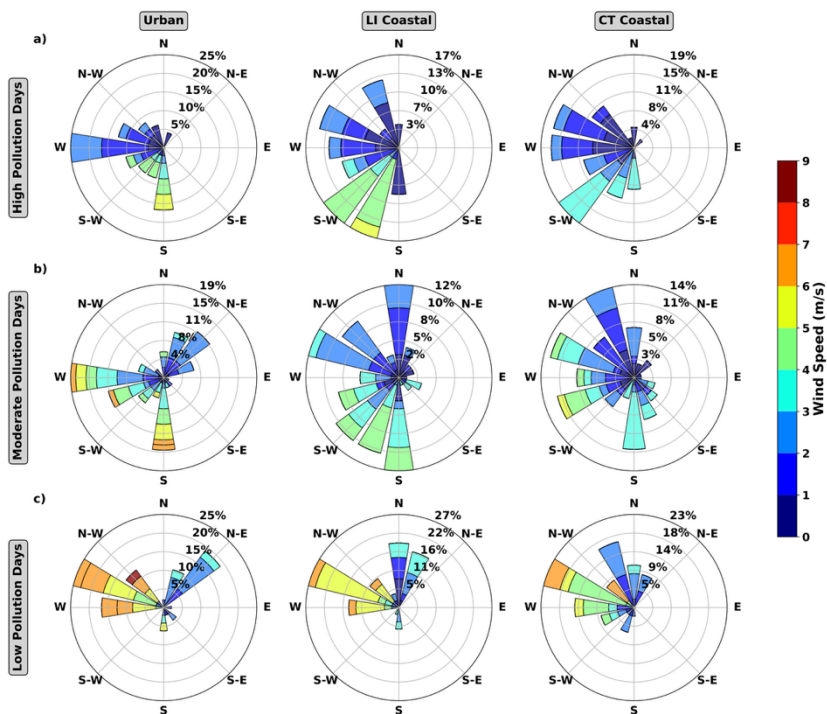


Figure S5: Wind roses of observed winds (m s⁻¹) for the three identified pollution cases: a) high, b) moderate, and c) low pollution organized by the three subregions: urban, LI coastal, and CT coastal. Note that the range of frequency of occurrence values shown in each figure panel differ.

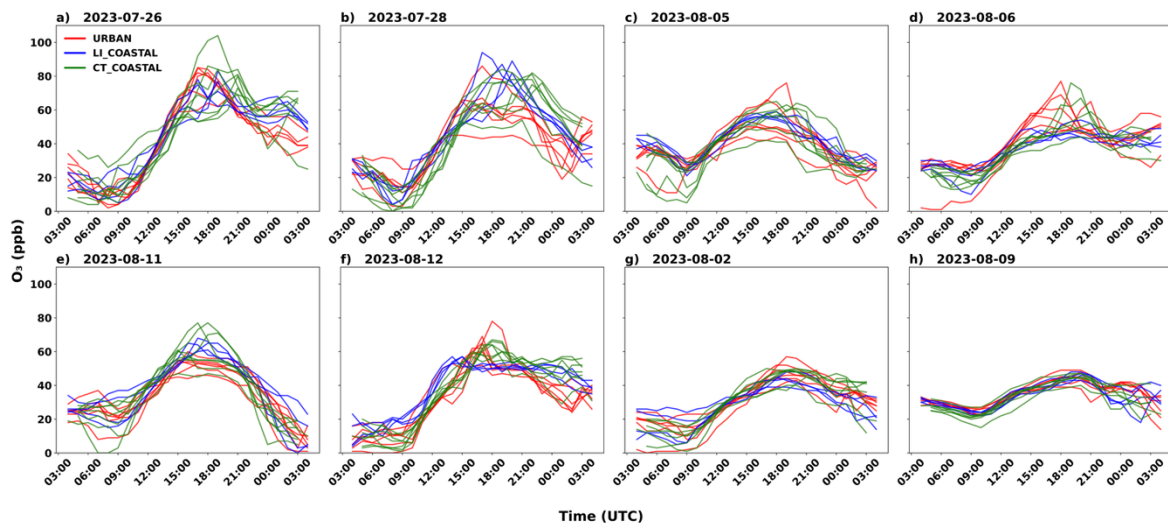


Figure S6: Observed surface O₃ (ppb) for all case days subset by region: urban sites (red), LI coastal (blue), and CT coastal sites (green). This figure provides additional detail complementing Figures 4, 7, S13, and S15 in the main text and supplementary text.

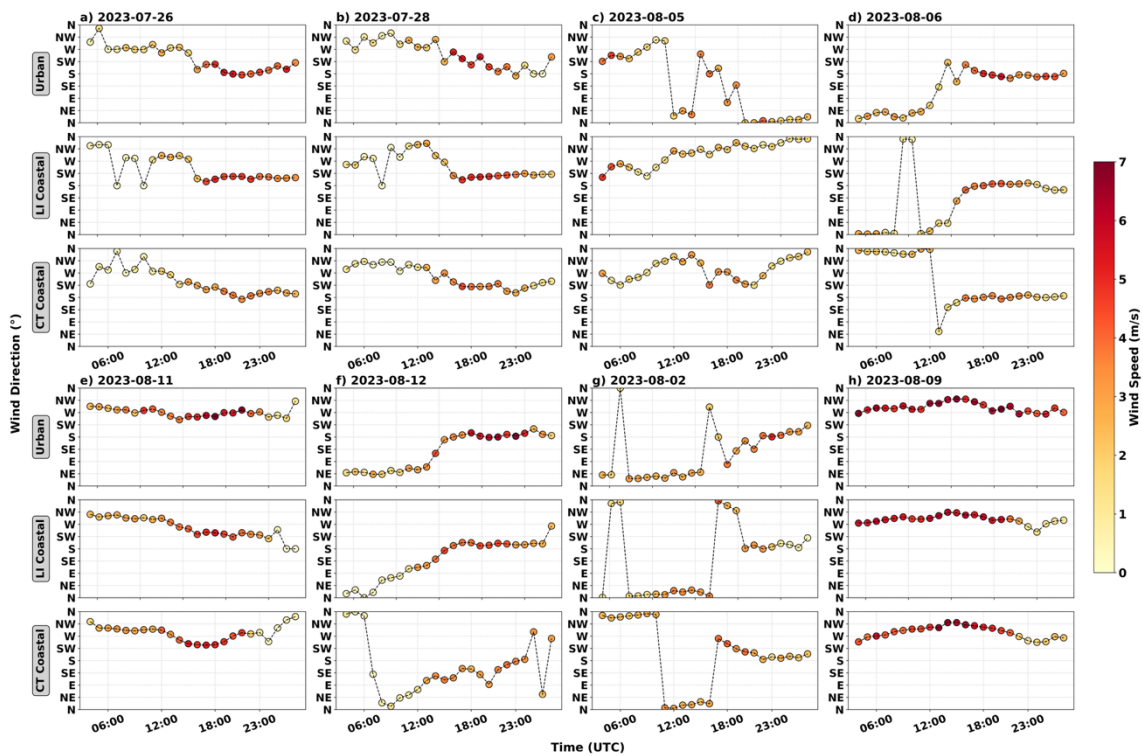


Figure S7: Observed average surface wind speed (m s^{-1}) and direction ($^{\circ}$) for all case days subset by region: urban sites, LI coastal, and CT coastal sites. This figure provides additional detail complementing Figures 4, 7, S13, and S15 in the main text and supplementary text.

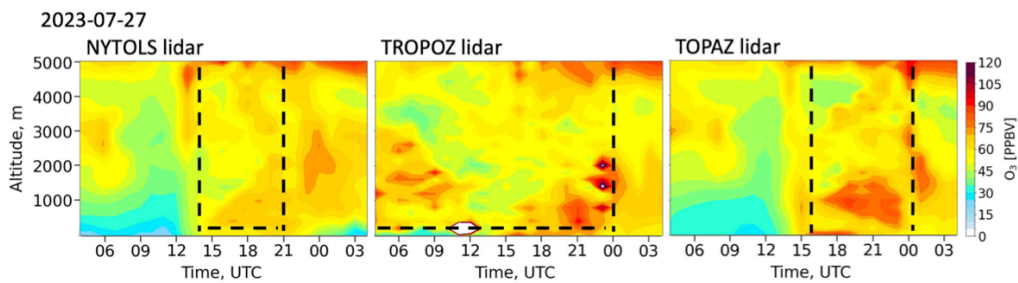


Figure S8. TOLNet lidar multidimensional O_3 (ppb) observations (outlined in black dotted lines) with WRF-Chem model simulated spatiotemporal O_3 filling missing data on July 27, 2023.

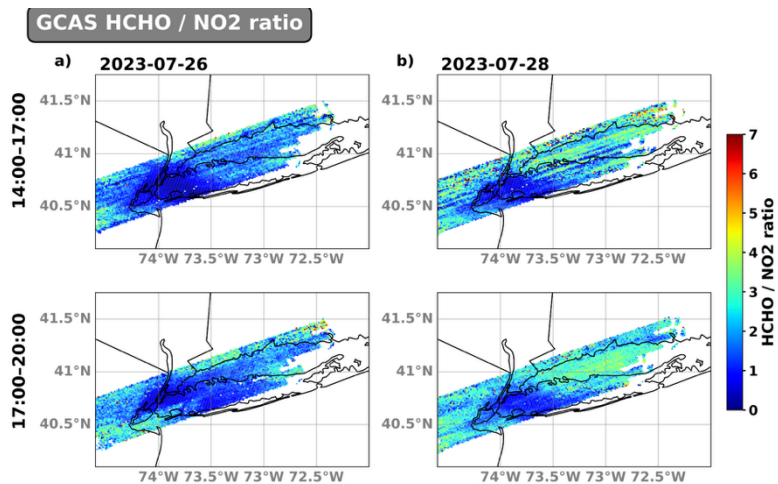


Figure S9. GCAS 3-hour averaged HCHO/NO₂ ratios on July 26 and 28, 2023.

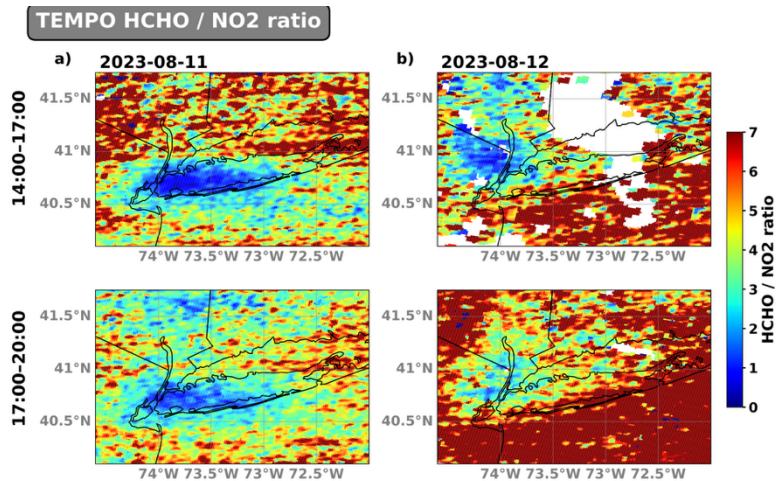


Figure S10. TEMPO 3-hour averaged HCHO/NO₂ ratios on August 11 and 12, 2023.

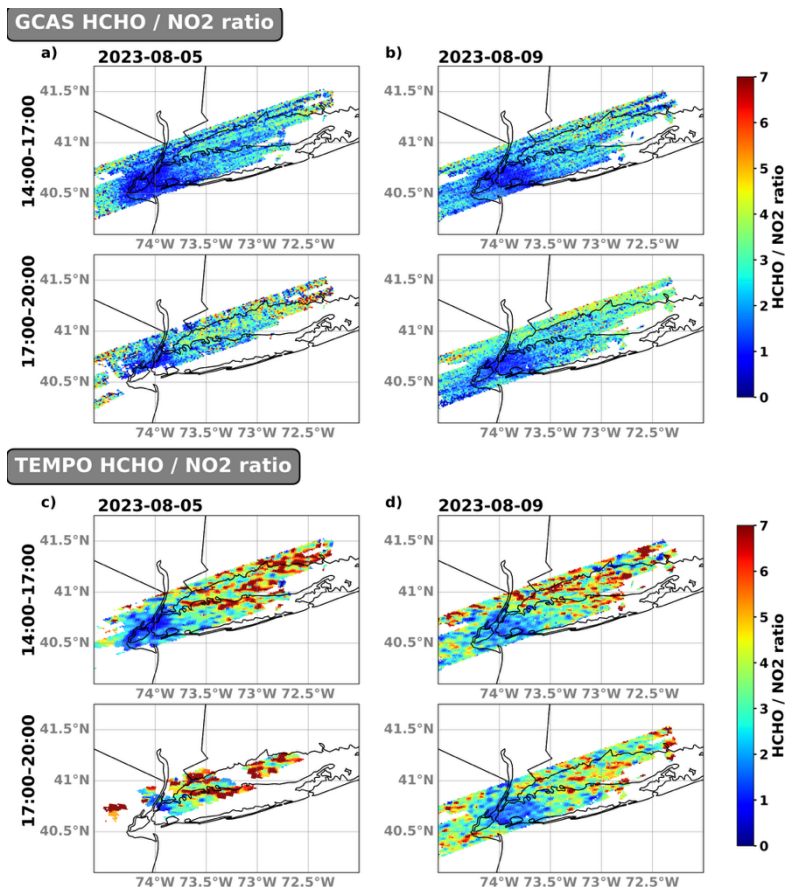


Figure S11. GCAS (a, b) and TEMPO (c, d) 3-hour averaged HCHO/NO₂ ratios on August 5 and 9, 2023.

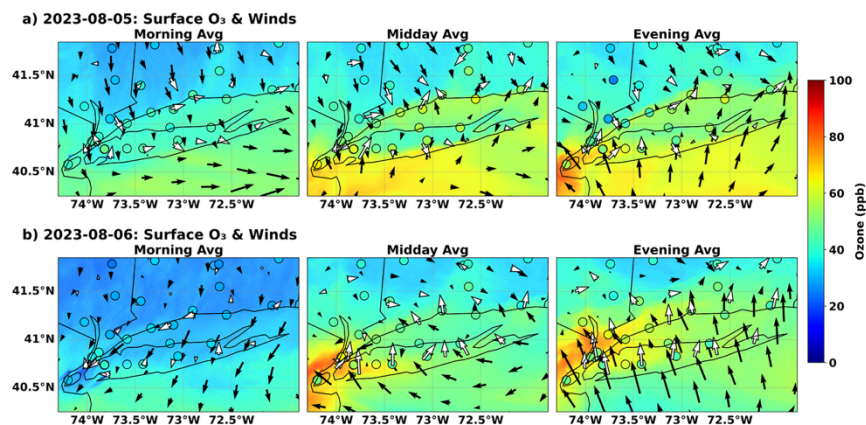
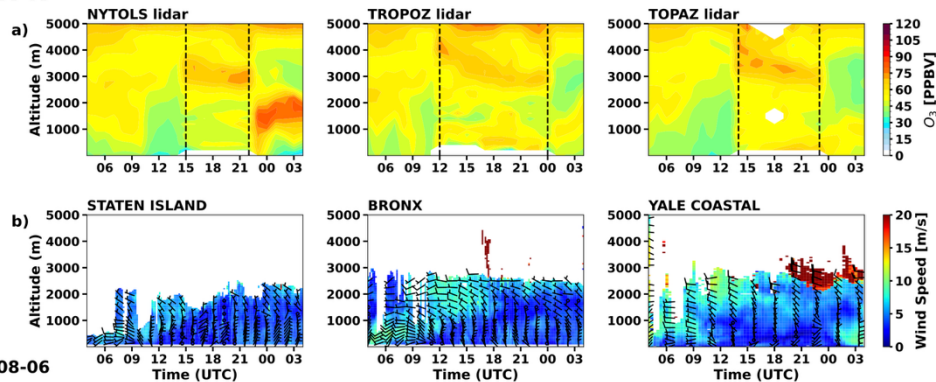


Figure S12. Morning, midday, and evening averaged AQS O₃ observations (scatter points) and ASOS winds (white arrows), overlaid with WRF-Chem simulated O₃ (contours) and winds (black arrows) for August 5 (a) and August 6, 2023 (b). Morning averages correspond to 11:00–15:00 UTC, midday to 15:00–19:00 UTC, and evening to 19:00–00:00 UTC.

2023-08-05



2023-08-06

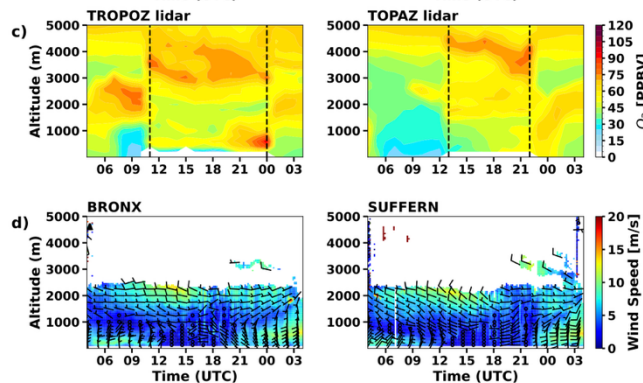


Figure S13. TOLNet lidar multidimensional O_3 (ppb) observations (outlined in black dotted lines) with WRF-Chem model simulated spatiotemporal O_3 filling missing data (a, c) and Doppler lidar (b, d) multidimensional wind profiles (m s⁻¹) observations at sites around NYC/LIS on August 5 and 6, 2023.

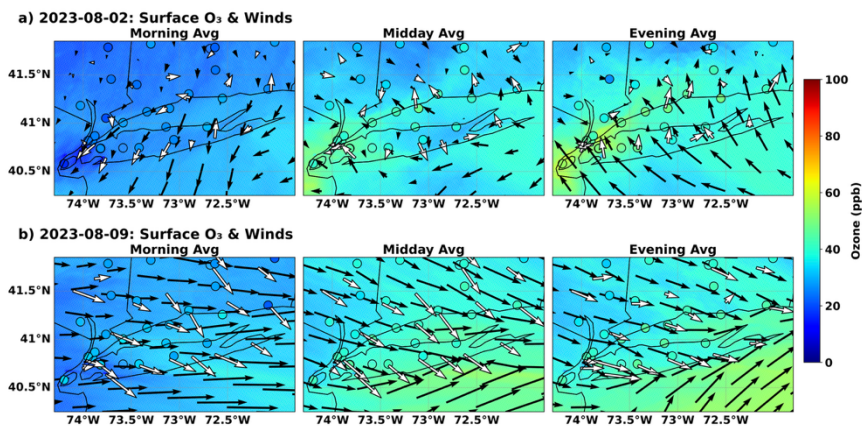
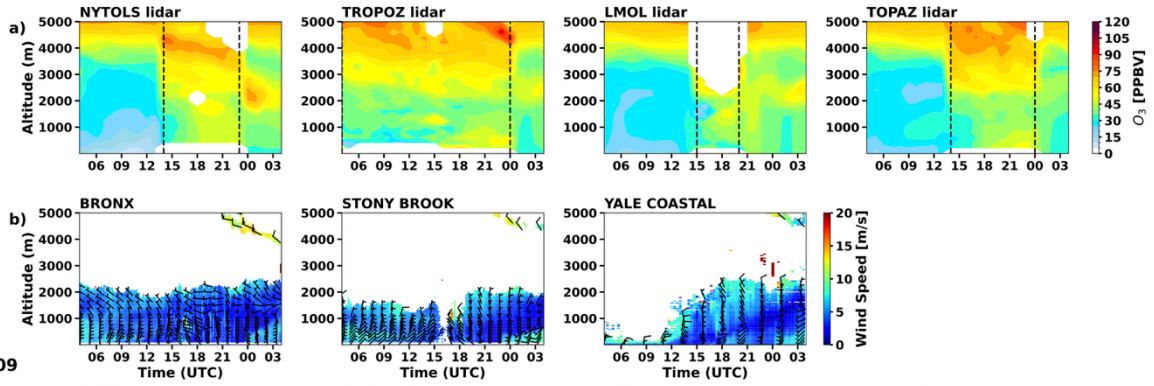


Figure S14. Morning, midday, and evening averaged AQS O_3 observations (scatter points) and ASOS winds (white arrows), overlaid with WRF-Chem simulated O_3 (contours) and winds (black arrows) for August 2 (a) and August 9, 2023 (b). Morning averages correspond to 11:00–15:00 UTC, midday to 15:00–19:00 UTC, and evening to 19:00–00:00 UTC.

2023-08-02



2023-08-09

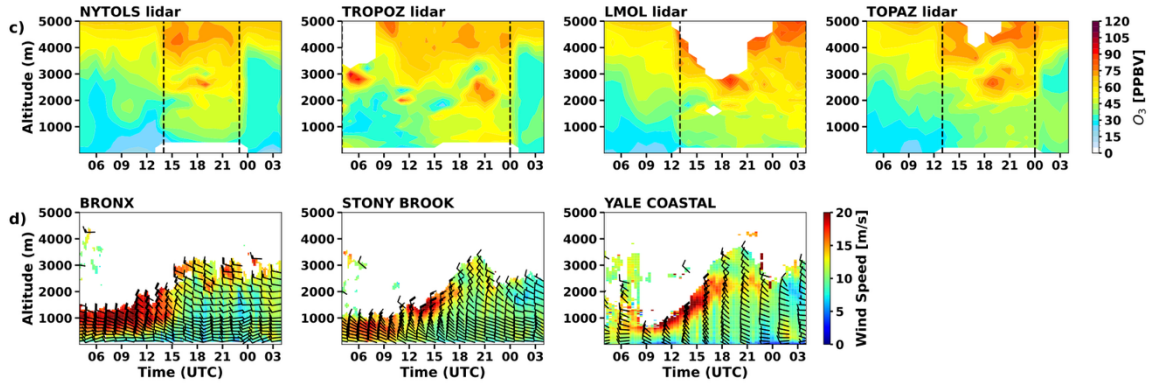


Figure S15. TOLNet lidar multidimensional O_3 (ppb) observations (outlined in black dotted lines) with WRF-Chem model simulated spatiotemporal O_3 filling missing data (a, c) and Doppler lidar (b, d) multidimensional wind profiles (m s⁻¹) observations at sites around NYC/LIS on August 2 and 9, 2023.

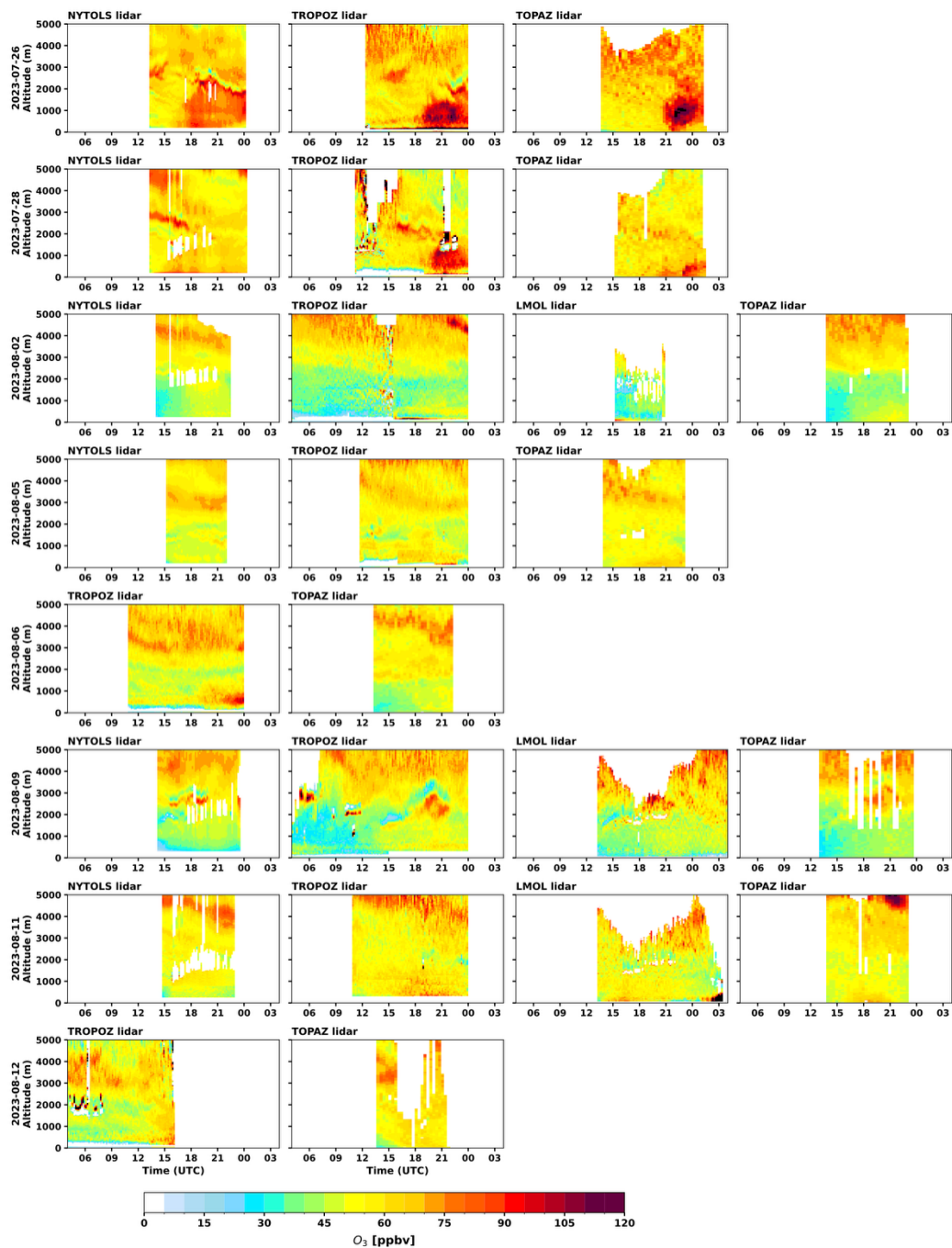


Figure S16. TOLNet lidar multidimensional O_3 (ppb) observations at original data retrieval quality for each day.