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Improving predictability of high-ozone episodes through dynamic boundary conditions, emission refresh and chemical data assimilation during the Long Island Sound Tropospheric Ozone Study (LISTOS) field campaign

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Table S1. Comparisons between LIS and NAQFC configurations during the LISLOS study.

Configuration	LIS	NAQFC
Horizontal resolution	3km	12km
Meteorology	WRF with Global Forecasting System (GFS) acting as ICs/BCs	North America Mesoscale Forecast System (NAM)
Lateral Boundary conditions	Various (Default/NAQFC)	Climatological gaseous LBC from GEOS-chem. Dynamic aerosol LBC from GEFS-Aerosol
Initial concentration	CMAQ restart file	Previous run
Base Emission	NEI2011v2	NEI2014v2
Chemistry	CB6 Aero6	CB05 Aero6

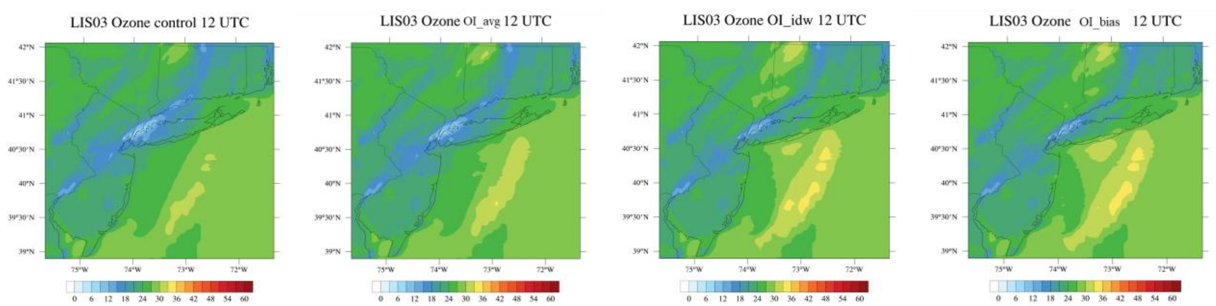

Figure S1: Spatial distributions of ozone simulated by Control, OI-avg, OI-idw and OI-bias at 0:00 and 12:00 UTC August 26, 2018.

Table S2: Regional mean statistical metrics between observed and simulated O_3 and NO_2 during the episode, the percentages indicated the rate of change compared to Control run from August 26 to 31, 2018.

Ozone	Control	BCON		NOAA		NO_2	Control	BCON		NOAA	
CORR	0.81	0.93	15%	0.91	12%	CORR	0.69	0.71	2%	0.67	-3%
RMSE	14.97	8.22	-45%	9.26	-38%	RMSE	4.12	3.82	-7%	4.98	21%
NMB	-0.3	0.14	52%	0.16	48%	NMB	-0.17	-0.06	-65%	-0.33	99%
NME	0.34	0.19	-45%	0.21	-38%	NME	0.35	0.33	-4%	0.43	23%

Extended daily forecasting run was also conducted during this research. The results showed the simulation without adjustment was able to predict the O_3 activities (Fig. S2b, e) while the concentration generally biased low. And the forecasting performance has been improved when applying these adjustments (Fig. S2c, f). It indicates this system also presented comparable performance during the non-episode time and has the potential to conduct the operational application after further adjustment.

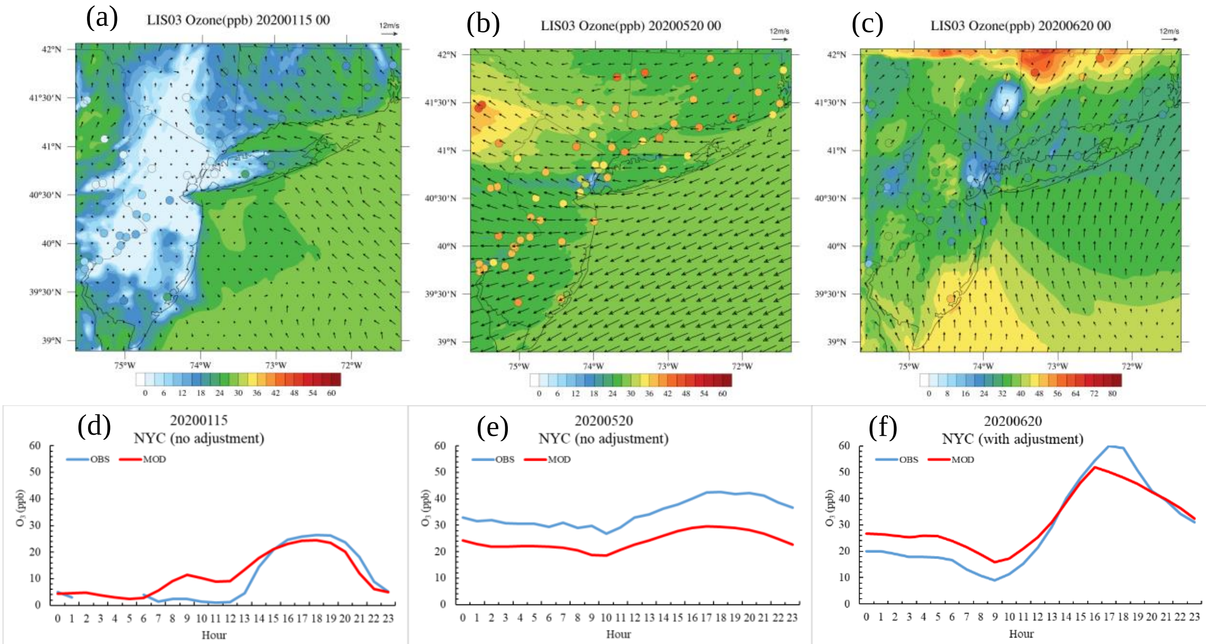

Figure S2: Spatial distributions diurnal variations of observed and simulated ozone on January 15 (a, d), May 20 (b, e) and June 20 (c, f), 2020.

Table S3: Statistical metrics between observed and simulated O_3 from Control run and OI_bias run in different sub-regions from August 26 to 31, 2018.

CORR	Control	OI_bias	RMSE	Control	OI_bias
NYC	0.78	0.82	NYC	16.26	14.89
PH	0.77	0.82	PH	15.67	14.68
HH	0.85	0.88	HH	13.55	12.38
PP	0.81	0.86	PP	17.12	15.18
OTHR	0.84	0.88	OTHR	12.24	11.46
Average	0.81	0.85	Average	14.97	13.72

Table S4: Statistical metrics of O_3 simulations after combined adjustment (dynamic BCs, ICs with OI-bias and emission refresh using EmisAdj_avg/EmisAdj_sub) in different sub-regions from August 26 to 31, 2018

	BOE (EmisAdj_sub)				BOE (EmisAdj_avg)			
	CORR	RMSE	NMB	NME	CORR	RMSE	NMB	NME
NYC	0.95	7.42	15%	17%	0.95	6.81	12%	15%
PH	0.93	9.20	20%	21%	0.93	9.35	20%	22%
NHH	0.93	8.49	15%	20%	0.93	8.62	16%	20%
PP	0.91	8.02	5%	15%	0.91	7.92	5%	15%
OTHR	0.97	8.19	21%	22%	0.97	8.14	21%	21%
Average	0.94	8.26	15%	19%	0.94	8.17	15%	19%

Table S5: Same with Table S4 but for NO_2

	BOE (EmisAdj_sub)				BOE (EmisAdj_avg)			
	CORR	RMSE	NMB	NME	CORR	RMSE	NMB	NME
NYC	0.84	3.81	-20%	25%	0.83	3.36	-10%	22%
PH	0.82	4.53	-23%	33%	0.82	4.71	-26%	34%
NHH	0.51	7.02	-33%	43%	0.52	7.18	-37%	44%
PP	0.69	2.77	-14%	35%	0.69	2.75	-11%	35%
OTHR	0.71	2.16	-21%	33%	0.71	2.17	-21%	33%
Average	0.71	4.06	-22%	34%	0.71	4.04	-21%	34%

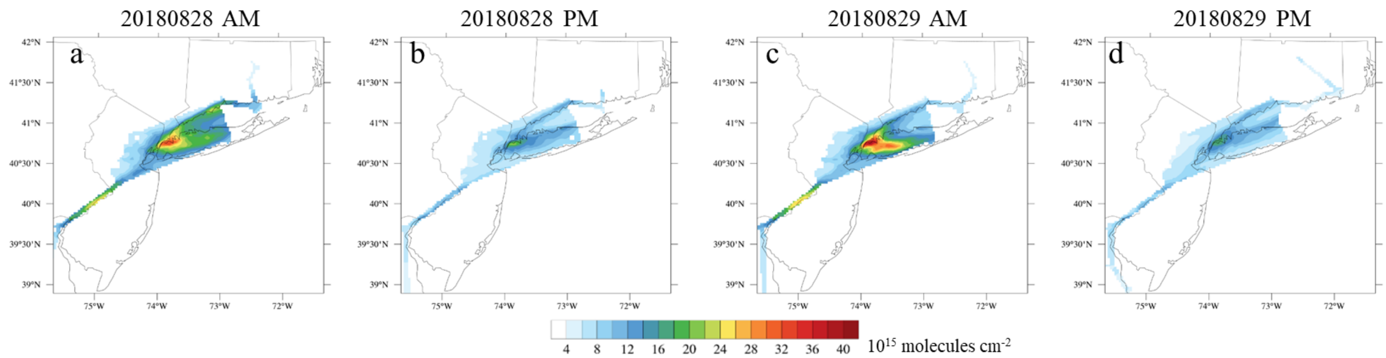

Figure S3: Spatial distribution of NO_2 vertical column density (VCD) simulated by the 3 km BOE (EmisAdj_sub) during August 28–29, 2018. There were two flight missions each day: the morning flight (AM) from ~11:00 to 15:00 UTC and afternoon flight (PM) from ~16:00 to 20:00 UTC.

Table S6: Statistical metrics between airborne measured and simulated NO_2 vertical column density on August 28 and 29, 2018

BOE (EmisAdj_avg)	CORR	NMB	NME	BOE (EmisAdj_sub)	CORR	NMB	NME	NAQFC	CORR	NMB	NME
28AM	0.56	69%	88%	28AM	0.57	60%	82%	28AM	0.44	48%	89%
28PM	0.81	44%	63%	28PM	0.81	34%	60%	28PM	0.79	76%	80%
29AM	0.79	25%	48%	29AM	0.79	20%	45%	29AM	0.41	12%	70%
29PM	0.78	23%	45%	29PM	0.79	16%	43%	29PM	0.65	44%	65%
Average	0.74	40%	61%	Average	0.74	33%	57%	Average	0.57	45%	76%

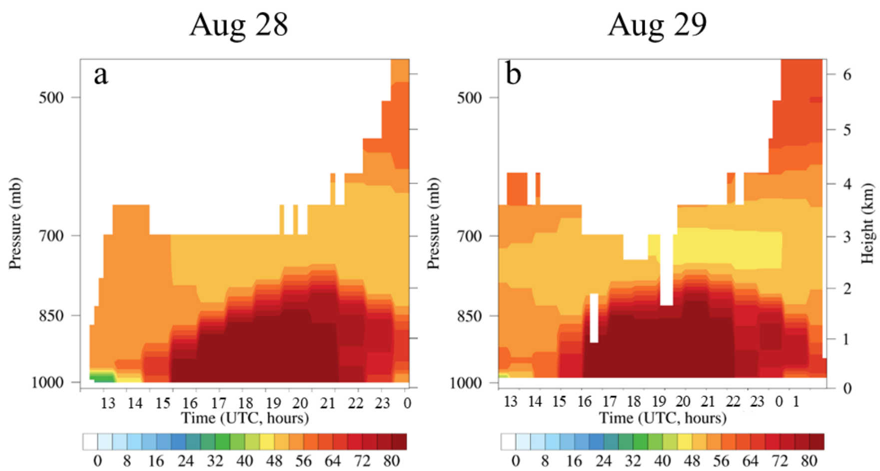

Figure S4: Vertical O_3 profiles simulated by the 3 km BOE (EmisAddj_sub) over the Westport site during (a) August 28 and (b) August 29, 2018.

Table S7: Statistical metrics between lidar measured and simulated O_3 profiles on August 28 and 29, 2018

	BOE(EmisAdj_avg)				BOE(EmisAdj_sub)				NAQFC			
	CORR	RMSE	NMB	NME	CORR	RMSE	NMB	NME	CORR	RMSE	NMB	NME
20180828	0.69	19.91	23%	27%	0.67	20.01	24%	28%	0.58	15.16	6%	21%
20180829	0.73	16.84	21 %	24%	0.72	16.74	21%	24%	0.50	17.86	12%	23%
Average	0.71	18.37	22%	26%	0.70	18.38	22%	26%	0.54	16.51	9%	22%

As there were limited measurements of isoprene in the LIS region, and the field campaign for VOC sampling occurred outside the study period. Instead, we compared the simulated hourly isoprene with AQS observations from a monitoring site in Bronx, NYC (Fig. S5). The predicted isoprene concentration agrees well with the observations regarding both levels and diurnal patterns, except underpredicting the peak values. The correlation coefficient is 0.93, higher than that of NO_2.

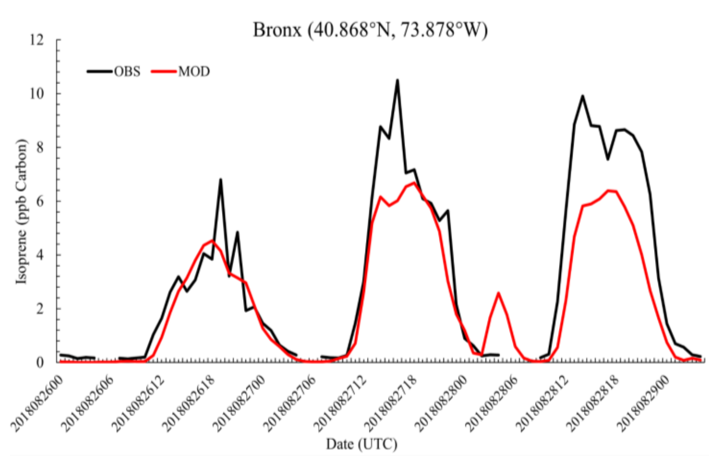

Figure S5. Observed and simulated hourly isoprene concentrations at Bronx, New York (40.868°N, 73.878°W) during the episode.