Improving ozone and nitrogen dioxide forecasting over the Long Island Sounds with dynamical boundary conditions, rapid emission refresh, and chemical data assimilation

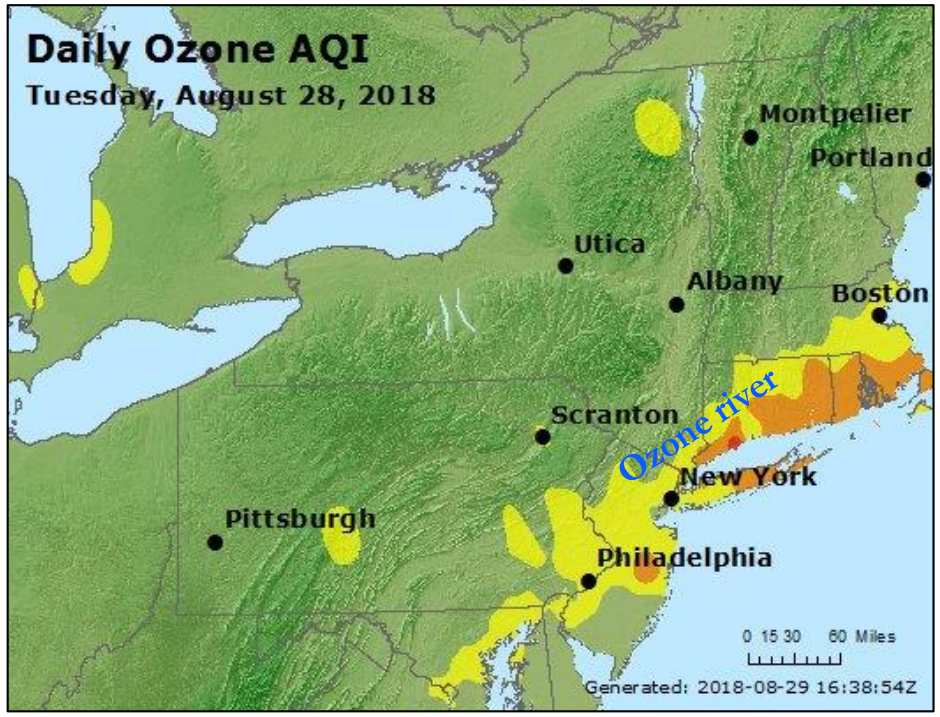
Siqi Ma[1], Daniel Tong[1,3], Lok Lamsal[2], Julian Wang[3], Youhua Tang[1,3], Tianfeng Chai[3], Pius Lee[3], Patrick Campbell[1,3], Barry Baker[1,3], Rick Saylor[3], Shobha Kondragunta[4], and Ivanka Stajner[5]

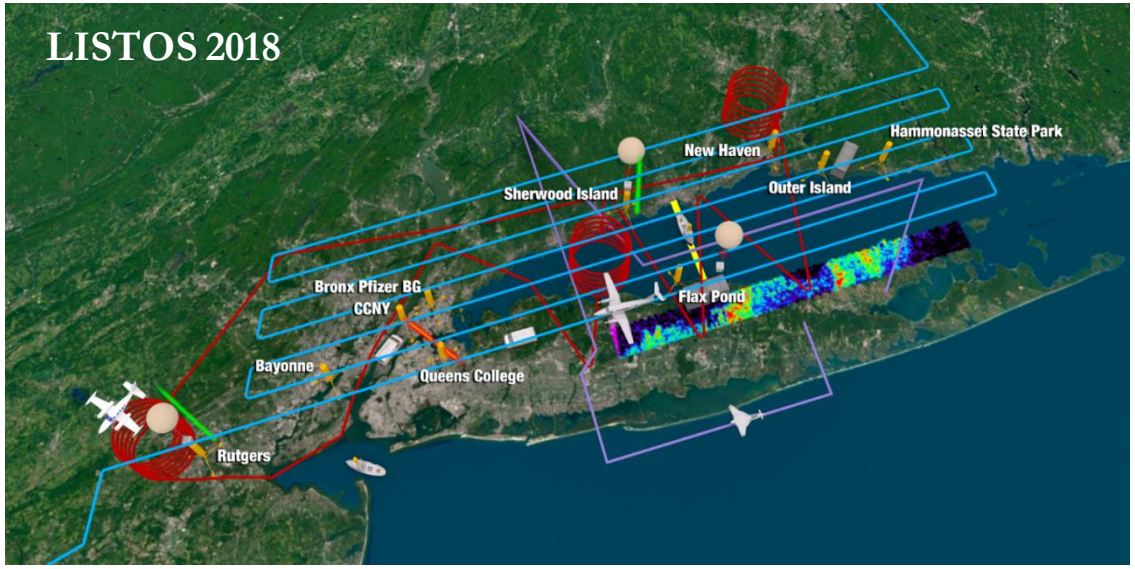
[1]George Mason University; [2]NASA Goddard Space Flight Center; [3] NOAA Air Resources Lab; 4 NOAA NESDIS/STAR; 5 NOAA NWS/NCEP

The 2020 CMAS Workshop, Chapel Hill, NC

How to Predict High Ozone in a Cleaner Urban Environment?

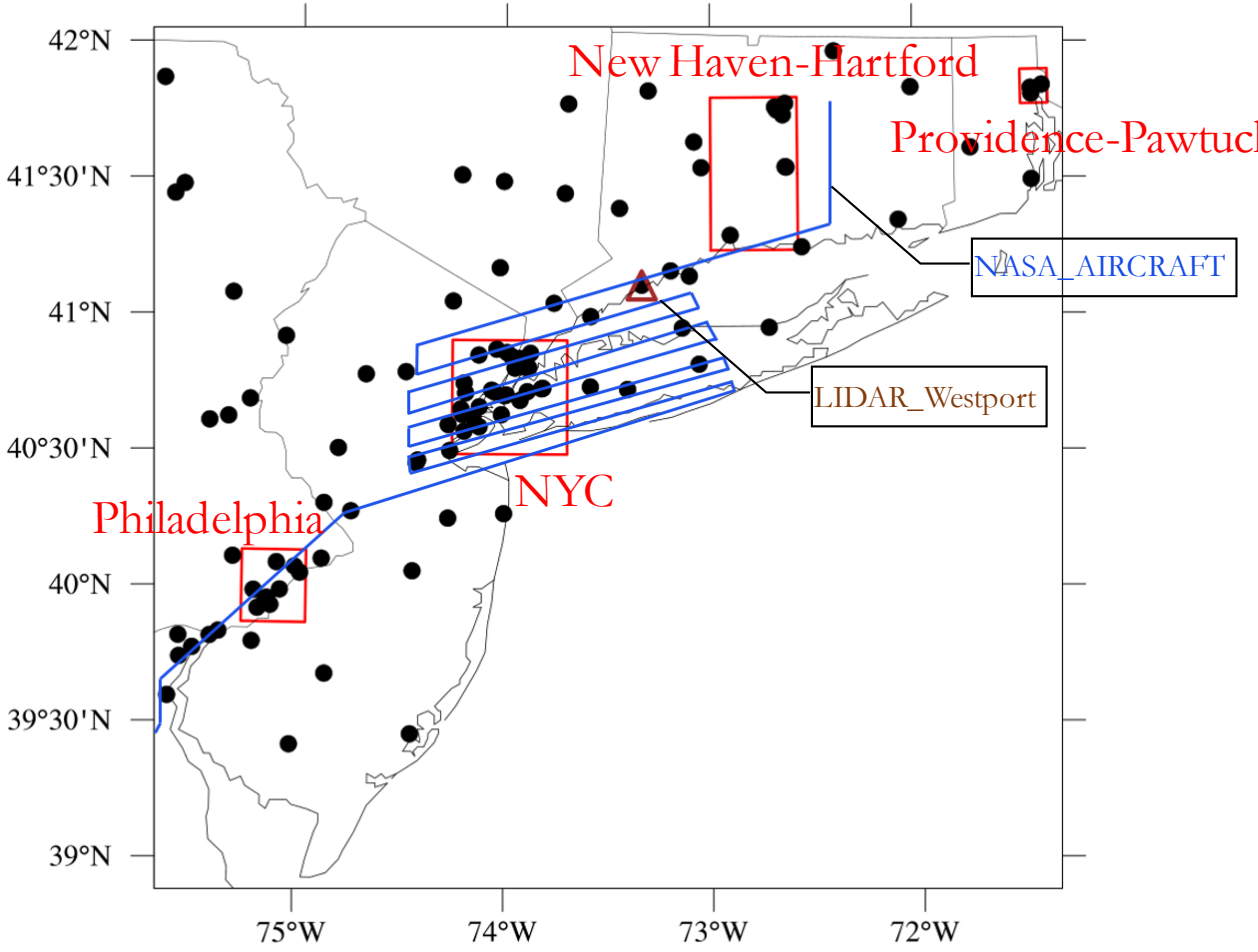
Long Island Sounds and Downwind areas continue to violate Ozone Standard regardless of improved air quality





The Long Island Sound Tropospheric Ozone Study 2018 provided various observational data collection to investigate the emission, chemistry, and meteorology in this region.

Study Domain and Observations



- Air Quality System (AQS) ground measurement
  - Hourly O_3 and NO_2
- Ozone Monitoring Instrument (OMI) aboard Aura satellite
  - Monthly NO_2 vertical column density (VCD), 0.1°
- LISTOS 2018 field campaign
  - NASA GeoTASO NO_2 VCD measurement
  - NASA Langley Mobile Ozone Lidar product

Study Design

Model configurations

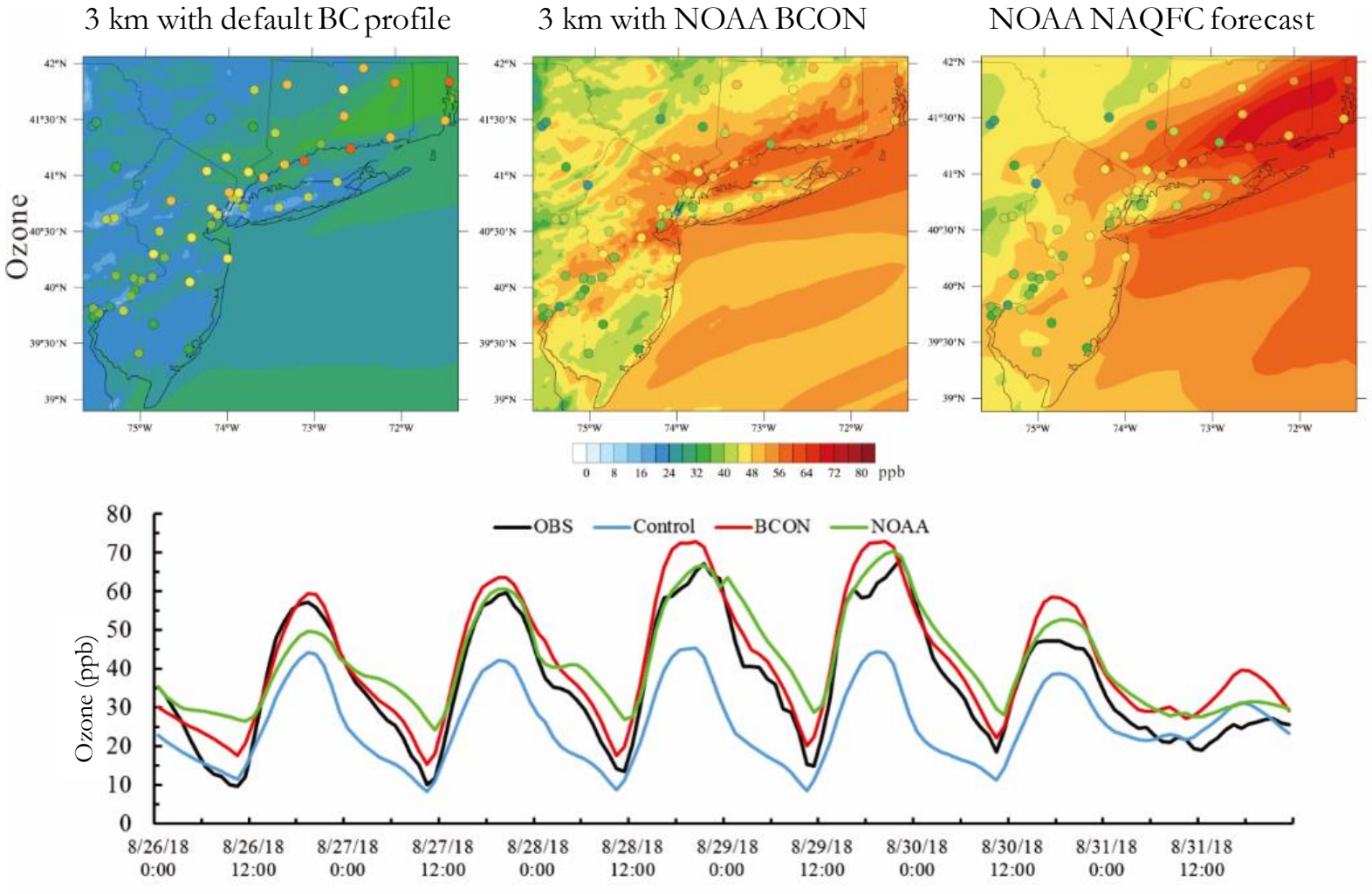
Model:	WRFv4.0 (CONUS suite)
	CMAQv5.3 (CB6 and AE6)
Date:	8.25~8.31, 2018
Resolution:	3×3 km
Vertical layers:	41 (20 below 1 km)
Meteorological:	Global Forecast System (GFS), 0.25° × 0.25°, 4/day
Emission:	US EPA 2011 NEI version 2 (NEI2011v2)
	Inline biogenic emission
	Inline sea-spray emission

Simulation settings

	Name	Adjustment
1	Control	Default configuration, profile BCs, unadjusted ICs and emission
2	BCON	NOAA NAQFC predictions act as dynamic BC
3	OI	CGRID adjustment with OI (**OI_avg**, **OI_idw**, **OI_bias**)
4	EmisAdj	NO_x emission projection from 2011 to 2018 (**EmisAdj_avg**, **EmisAdj_sub**)
5	Combined	Combination of the adjustment methods. **BCON+OI (BO)**, **BCON+OI+EmisAdj (BOE)**

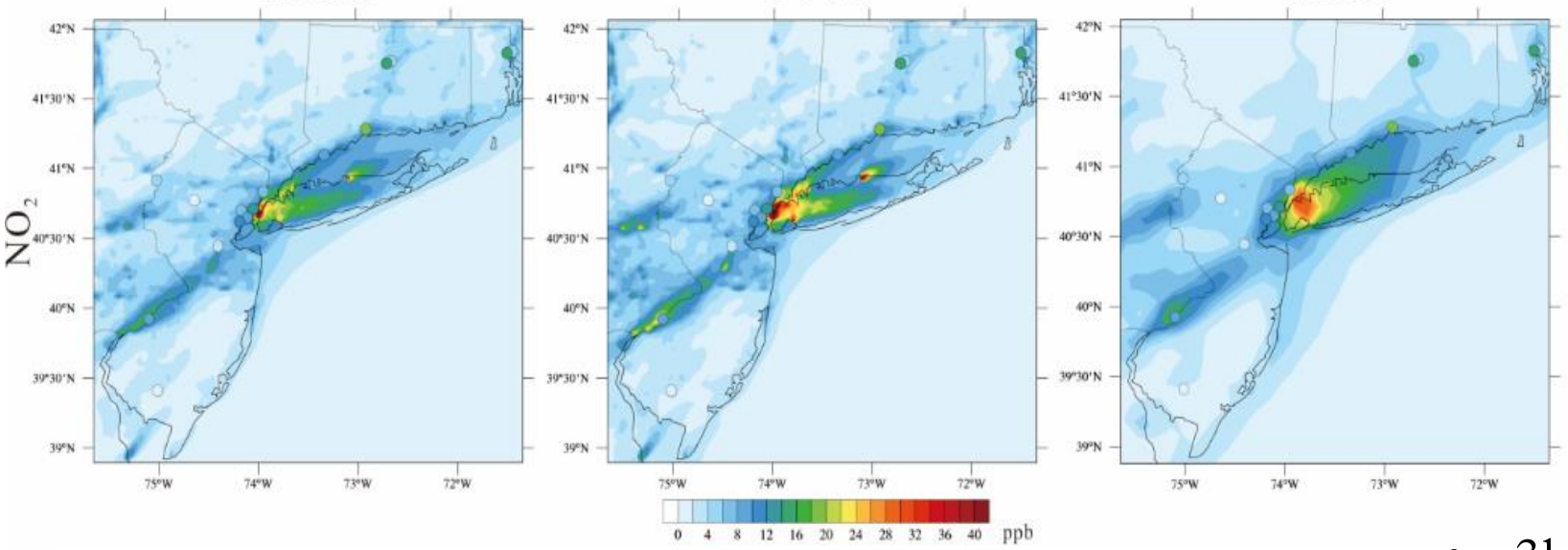
Effects of Boundary Conditions on O_3 Prediction

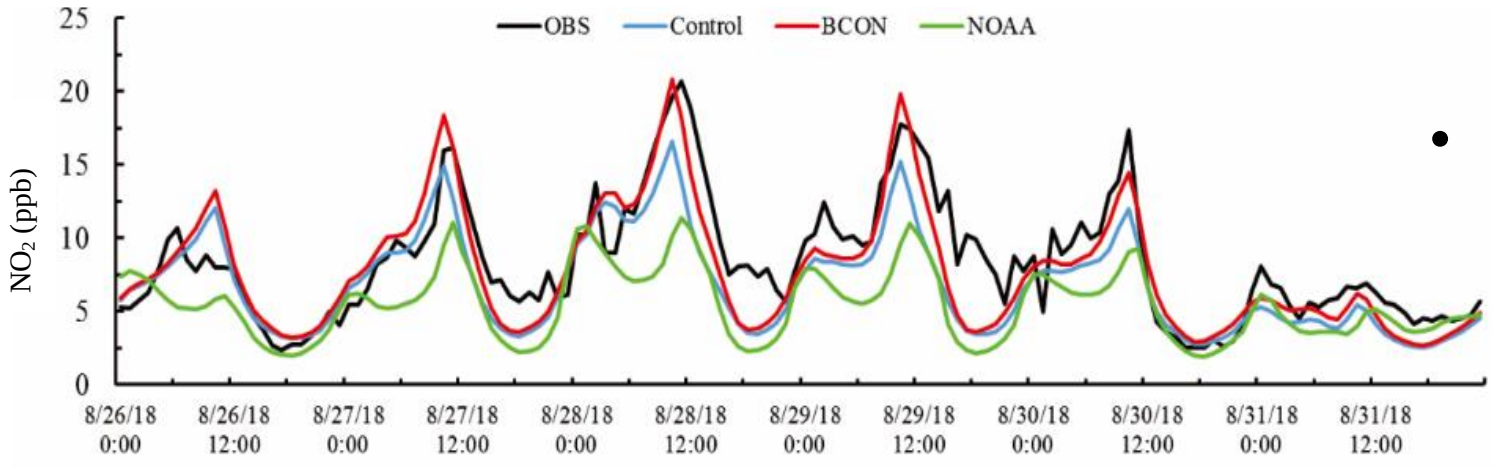
Daily O_3 on August 29, 2018



Effects of Boundary Conditions on NO_2 Prediction

3 km with default BC profile 3 km with NOAA BCON NOAA NAQFC forecast

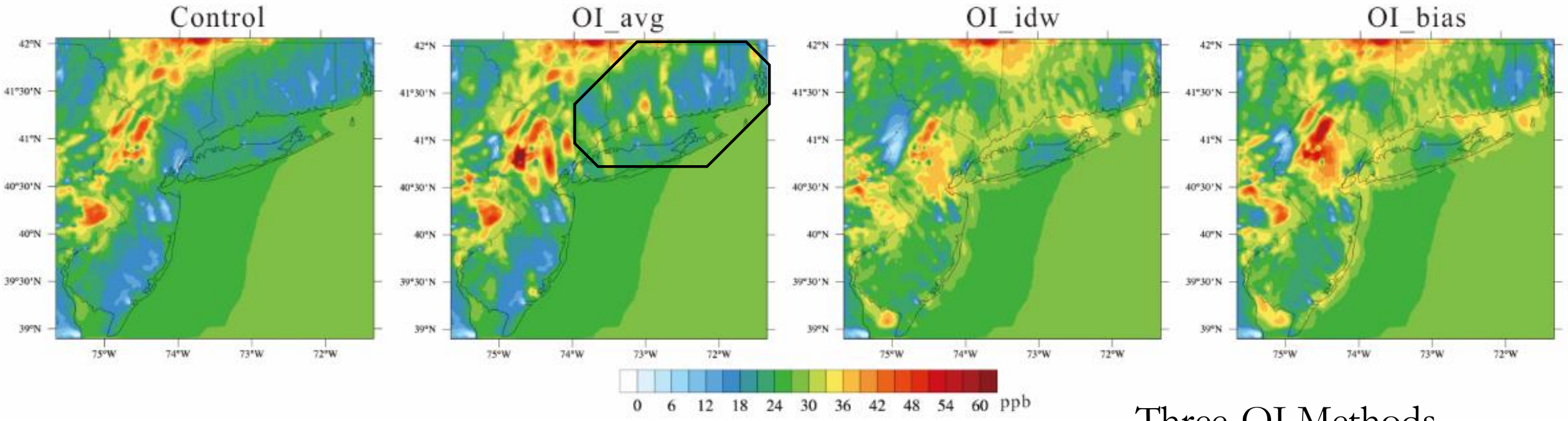




- 3km Run outperforms NAQFC in both cases;
- Best Performance: 3km with NAQFC BCON.

Effects of Initial Condition Adjustment
(Optimal Interpolation or OI)

O_3 distribution at 0:00 UTC August 26, 2018

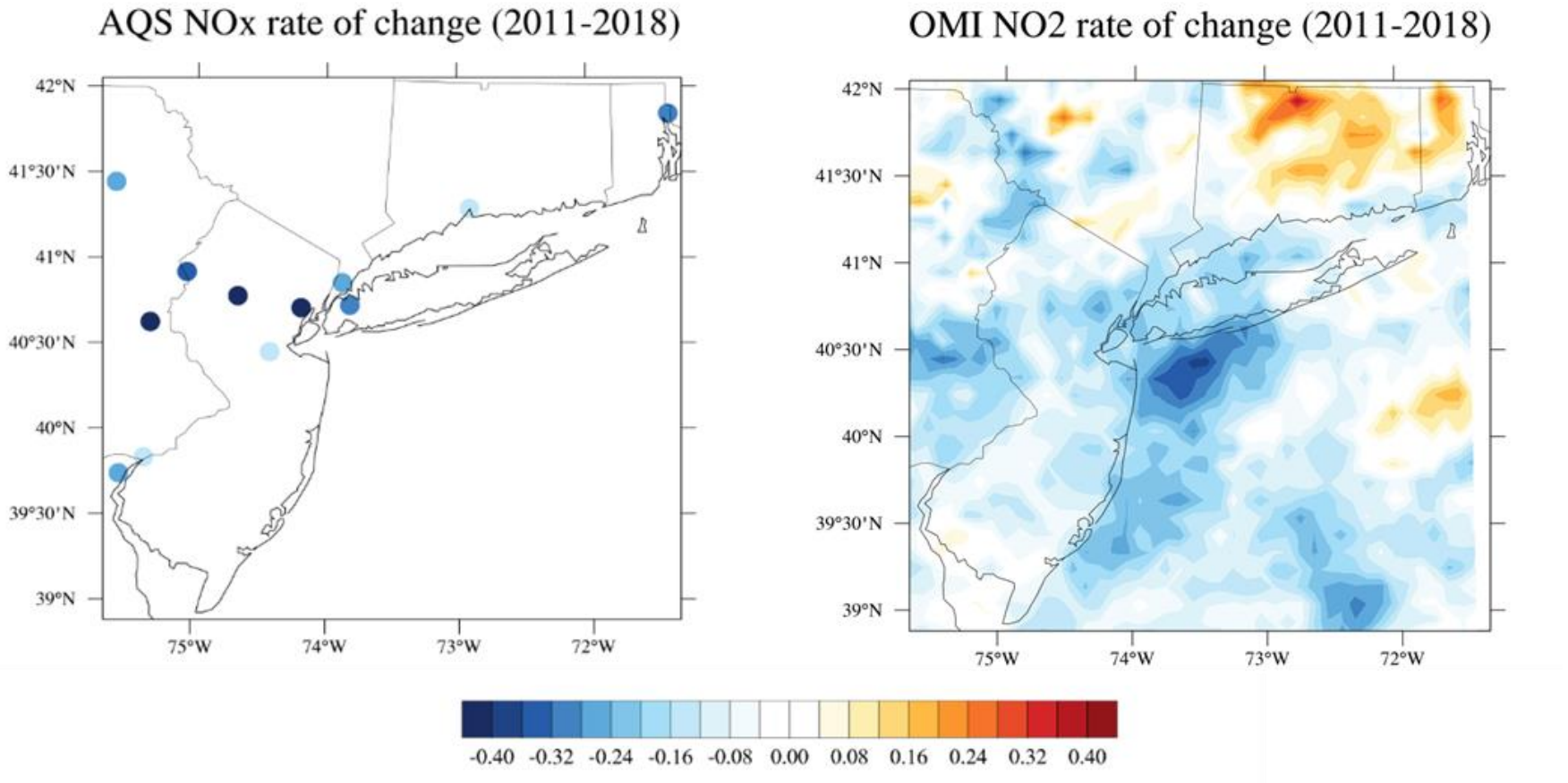


In the first 12 h, ozone performance enhanced with a mean CORR of 0.91 (0.83 for Control run) while during the last 12 h the CORR is only 0.8.

Three OI Methods

Stats\Runs	Control	OI_avg	OI_idw	OI_bias
CORR	0.81	0.84	0.86	0.86
RMSE	14.97	13.96	13.01	12.92
NMB	-0.30	-0.28	-0.25	-0.24
NME	0.34	0.32	0.29	0.29

Effects of NO_x Emission Adjustment

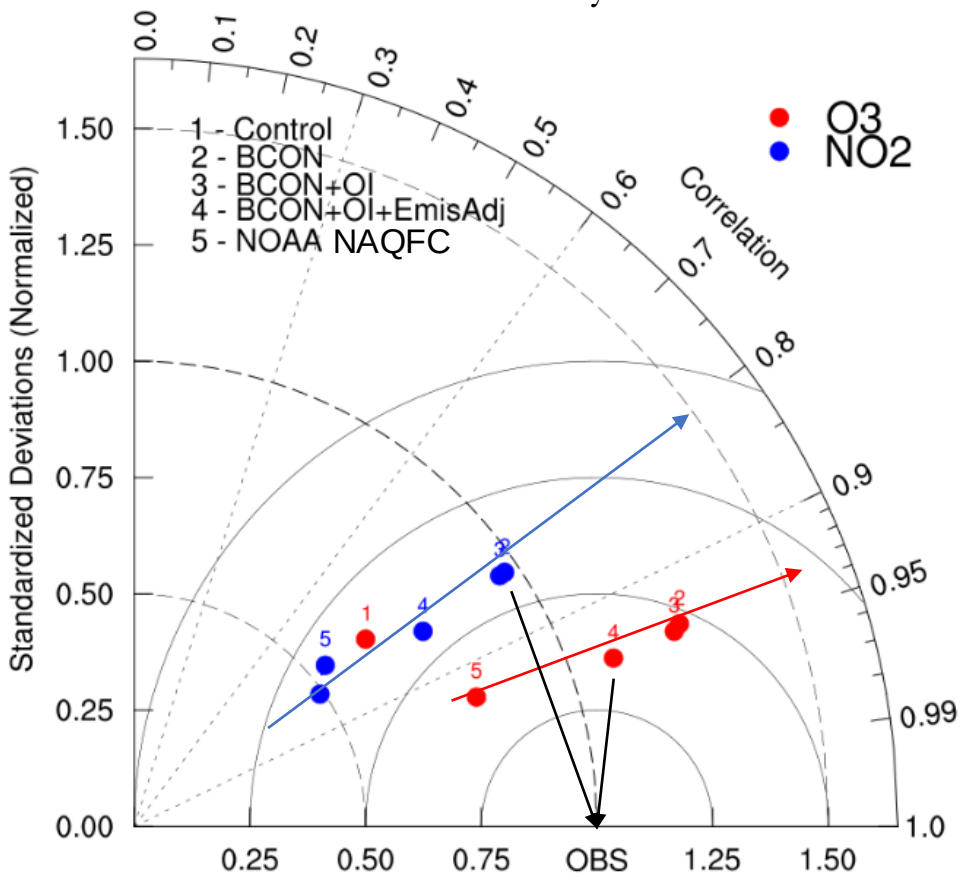


Interestingly, emission adjustment improves O_3 prediction but not NO_2 prediction.

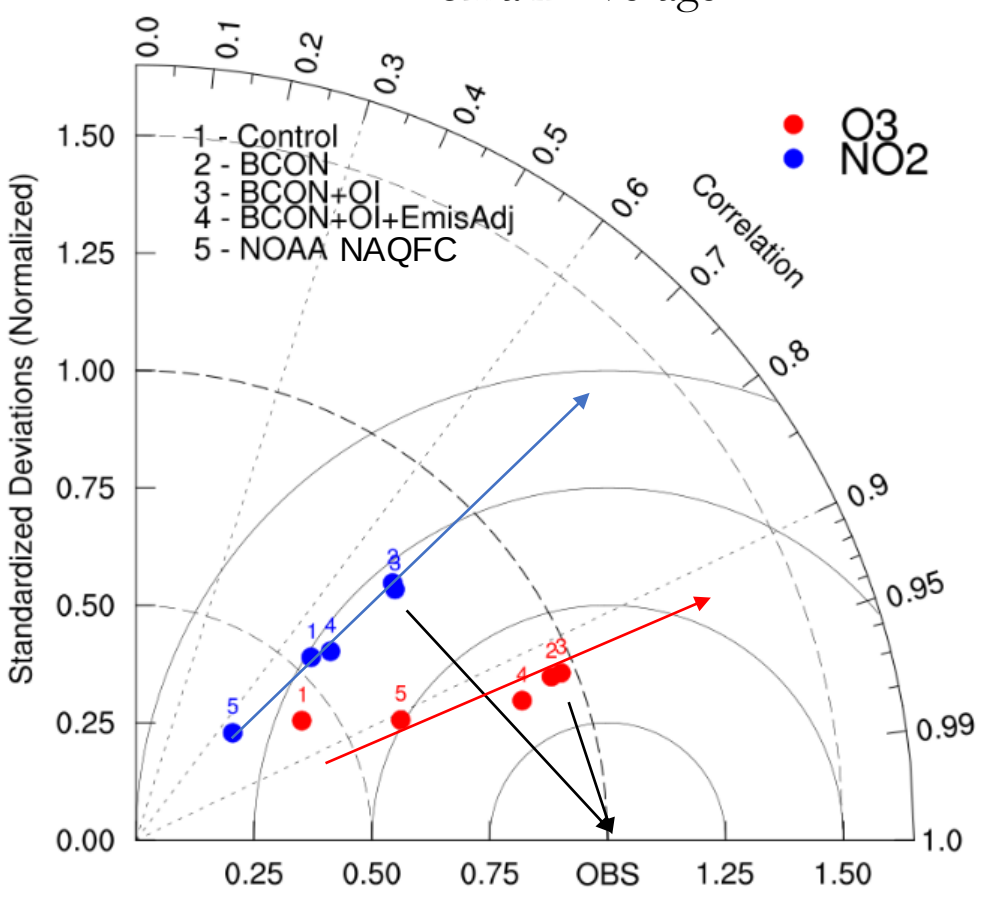
Effectiveness of Forecasting Techniques

- Control – 3km run without adjustment;
- BCON – 3km run with NAQFC BCON;
- BCON+OI – 3km run with BCON plus OI;
- BCON+OI+EmisAdj – 3km run with BCON, OI and Emission Adjustment all implemented;
- NOAA NAQFC – NAQFC Forecasting (12km).

New York City



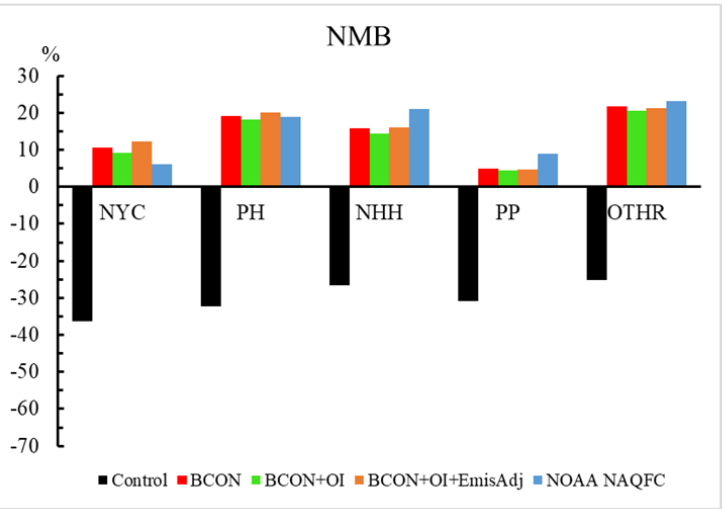
Domain Average

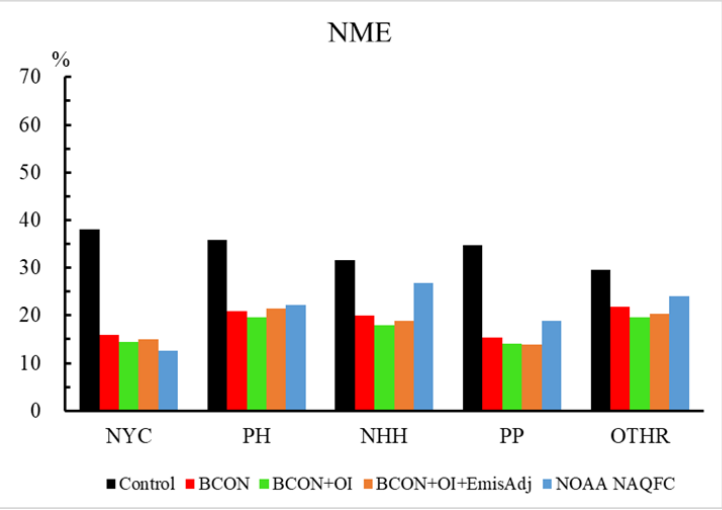


Effectiveness of Forecasting Techniques

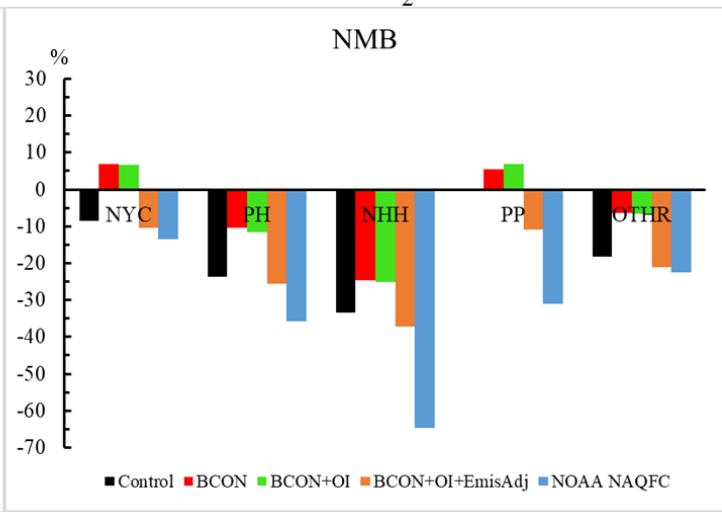
Statistical Metrics: Normalized Mean Error (NME)
Normalized Mean Bias (NMB)

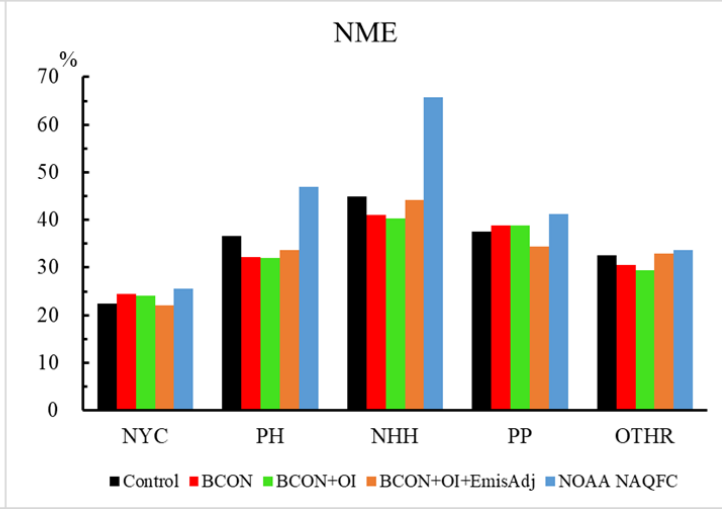
Ozone





NO_2



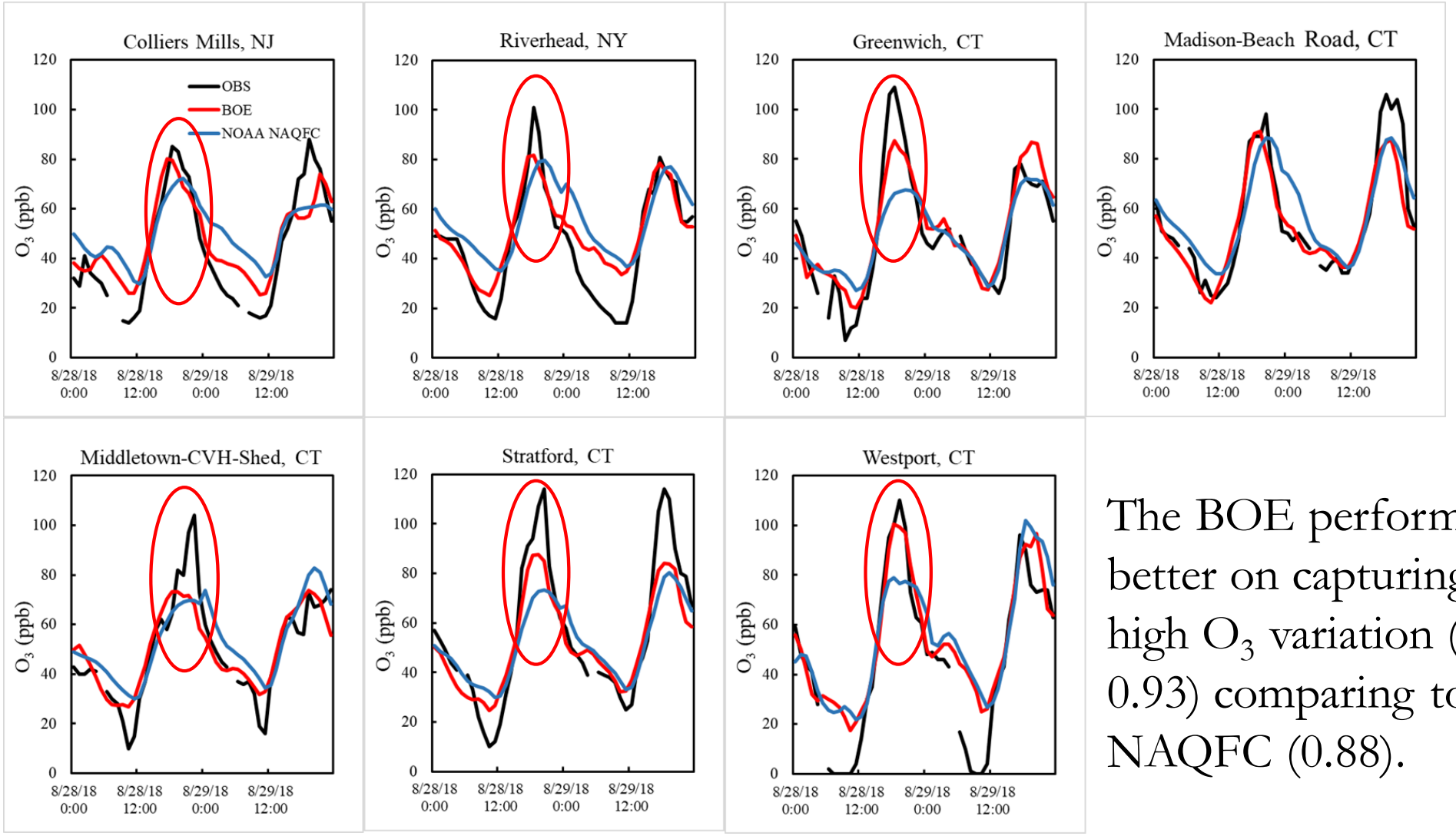


- NO_2 improvement not as significant as O_3.
- Simulations with combined adjustment have better performance.
- NOAA NAQFC performs well on O_3 while underestimates NO_2.

For surface performance:
BO > BOE > BCON > NAQFC > Control

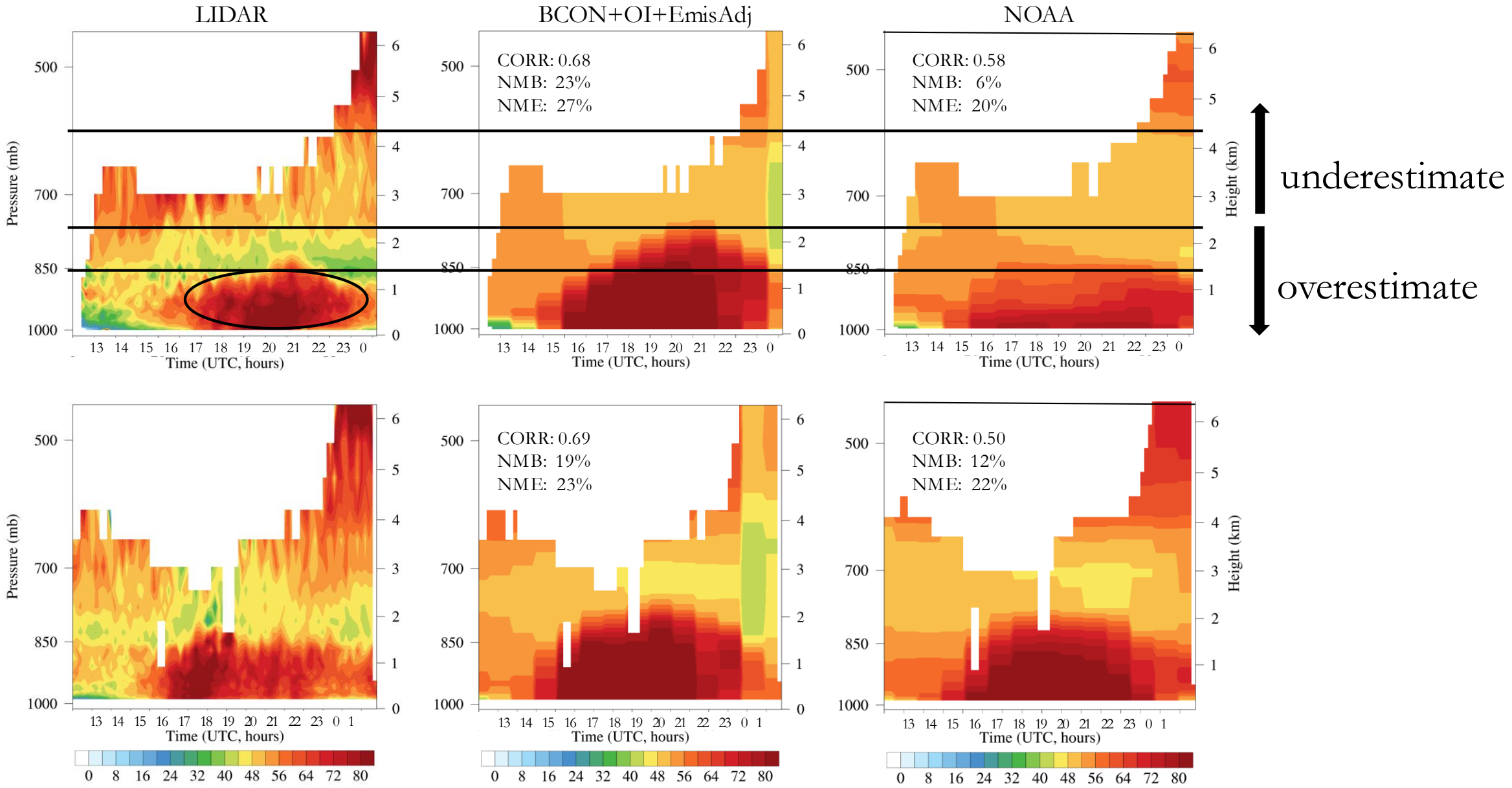
High Ozone Episode during LISTOS

O_3 time series at nonattainment sites during the episode (Aug 28~29, 2018)



The BOE performed better on capturing the high O_3 variation (CORR: 0.93) comparing to NAQFC (0.88).

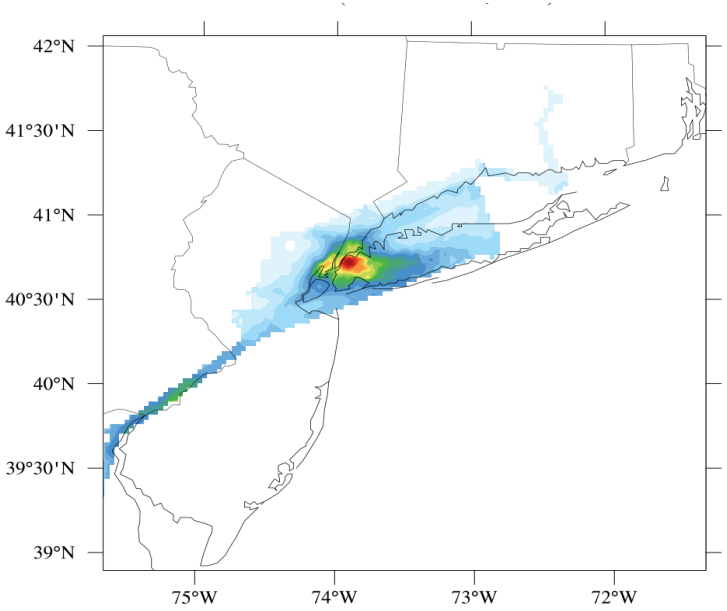
Vertical O_3 Profile



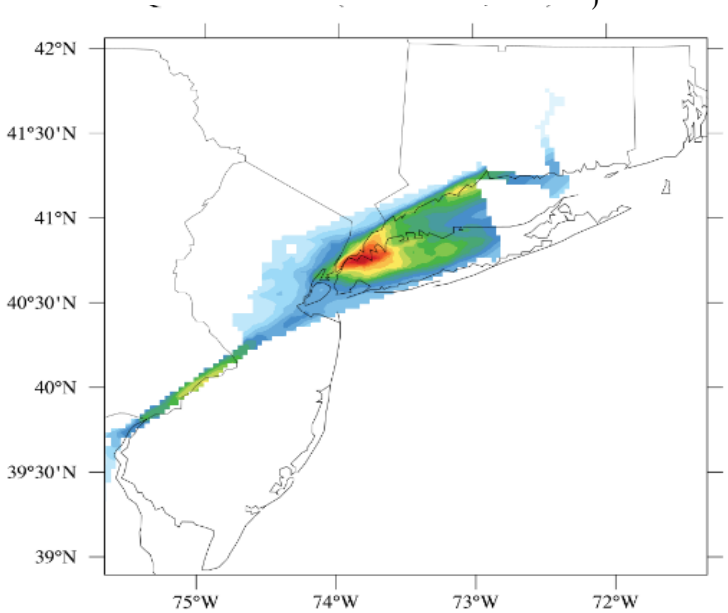
NO_2 Column Density: CMAQ vs GeoTASO

20180828 AM (~11:00 to 15:00 UTC)

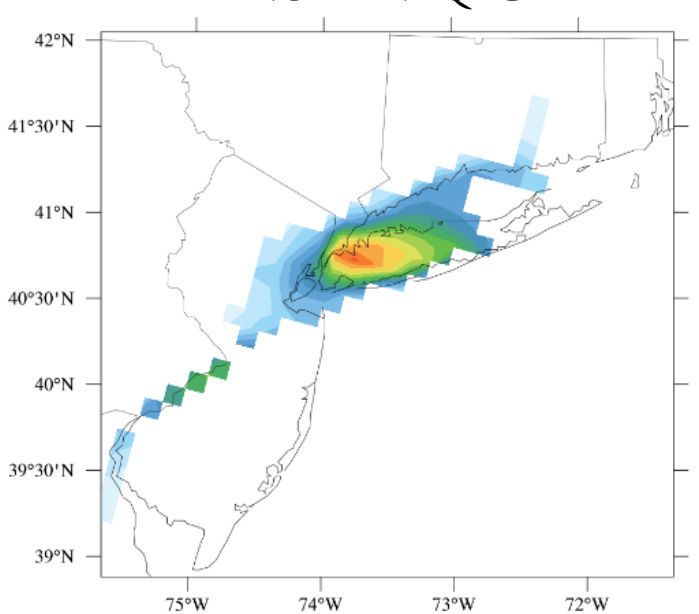
Aircraft

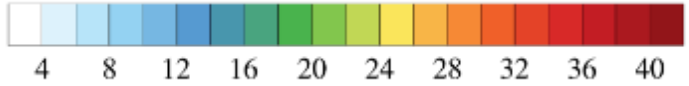


BCON+OI+EmisAdj



NOAA NAQFC





10^{15} molecules cm^{-2}

Statistics:	**NAQFC**	**3km(BOE)**
CORR:	0.59	0.73
NMB:	68%	62%
NME:	92%	76%

Conclusion

1. The 3km run always outperforms NAQFC (12km) for NO_2 prediction;
2. Dynamic boundary conditions derived from NOAA NAQFC is critical for the 3km O_3 prediction.
3. Chemical and emission data assimilation both enhance O_3 prediction, but with mixed results for NO_2.
4. Best performer during high O_3 events is the 3km run equipped with NAQFC boundary conditions, emission and chemical data assimilation.