

# A high-resolution modeling study of a heat wave- driven ozone exceedance event in New York city and surrounding regions

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# Outline

- ❖ Motivation and Objectives
- ❖ Model and Data
- ❖ Results and Discussion
- ❖ Summary
- ❖ Future work

# Motivation

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- ❖  $O_3$  is one of the major air pollutants in New York and surrounding areas.
- ❖ **Heat wave** is defined as the daily maximum temperature higher than  $32\text{ }^\circ\text{C}$  and **last for more than three days**, and is one of the **major factors causing  $O_3$  exceedance events (daily 8-hr max  $> 70$  ppb)** in **this region**.
- ❖ **High temperature and relevant meteorological factors** are one of the major contributors to unusually high  $O_3$  concentrations during the heat wave events (Pu et al., 2017; Fiala, 2003; Emberson et al., 2003; Wu et al., 2017).

# Motivation (cont.)

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- ❖ The conventional measurements are not sufficient to quantify the impact of heat wave on ozone exceedance events, and numerical models are useful for better **understanding** the mechanisms for the regional transport and local chemical productions. (Eric Chaxel et al., 2009) .
- ❖ New York has complex urban terrain and easily affected by the land-sea breezes. It is important to predict O<sub>3</sub> exceedance events with a high-resolution numerical model which includes the urban land surface processes.
- ❖ It is critical to utilize high resolution of numerical model(s) for improving air quality forecasting in a coastal megacity like New York.

# Objectives

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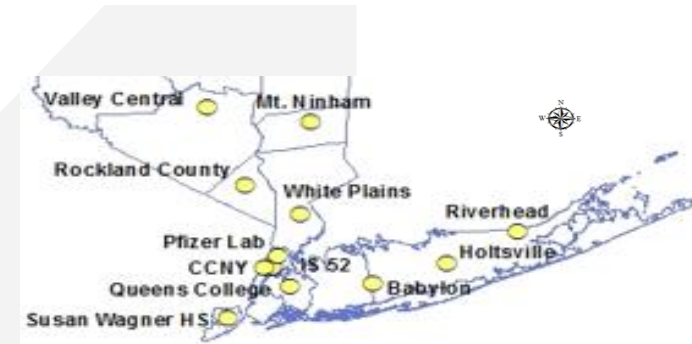
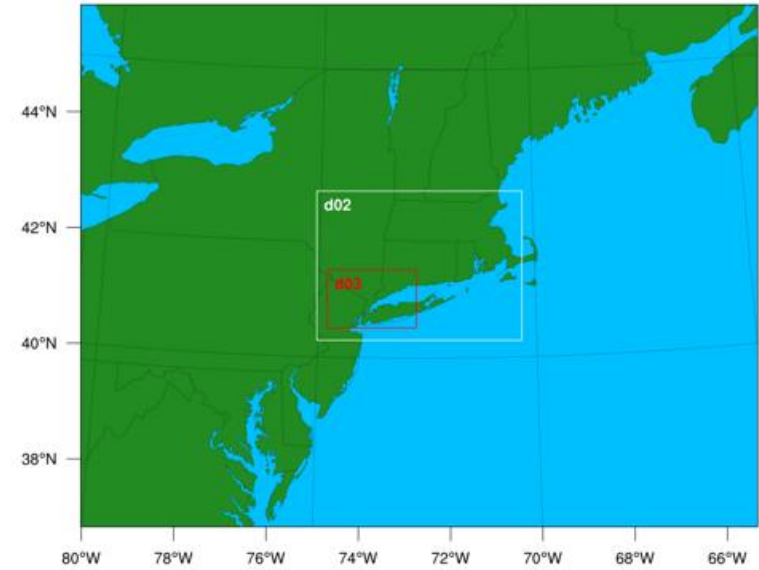
- ❖ to improve air quality forecasting especially for ozone exceedance events with **high-resolution** simulations.
- ❖ to **quantify the contributions** of chemical reactions associated with heat waves to ozone production during a heat wave-driven ozone exceedance event.

# Model and Data

## ❖ WRF-Chem

**Table 1 Parameter settings in WRF-Chem model**

Domain	1,2,3
Version	3.7.1
Time	16May 2017 to 20 May 2017
Initial Meteorological Field	Fnl (1°×1°) time: 6h 26 levels in vertical (1000hPa to 10hPa)
Horizontal Resolution	12km 4km 1.333km
P-Top	50 hPa
Horizontal Grid Point	110×85 100×73 88×61
Vertical Layers	46



**Fig. 1 Nested domains of WRF-Chem and observational sites.**

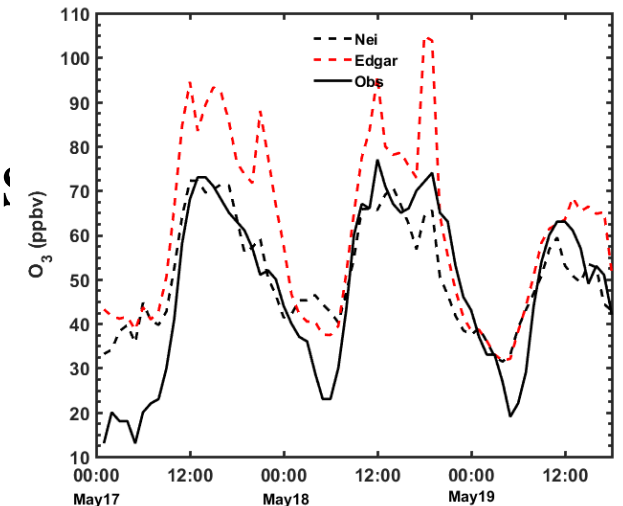
# Model and Data (cont.)

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- Initial and boundary conditions for chemical fields in WRF-Chem are generated from the MOZART-4/GEOS-5 simulations (<http://www.acd.ucar.edu/wrf-chem/mozart.shtml>)
- Meteorological ICs and BCs are from the NASA GMAO GEOS-5 simulations
- Horizontal resolution :  $1.9^{\circ} \times 2.5^{\circ}$
- Vertical : 56 layers
- Anthropogenic emissions based on David Streets' inventory for [ARCTAS](#) and the fire emissions from FINN-v1 (Wiedinmyer et al., Geosci. Model Devel, 2011).

# Model and Data (cont.)

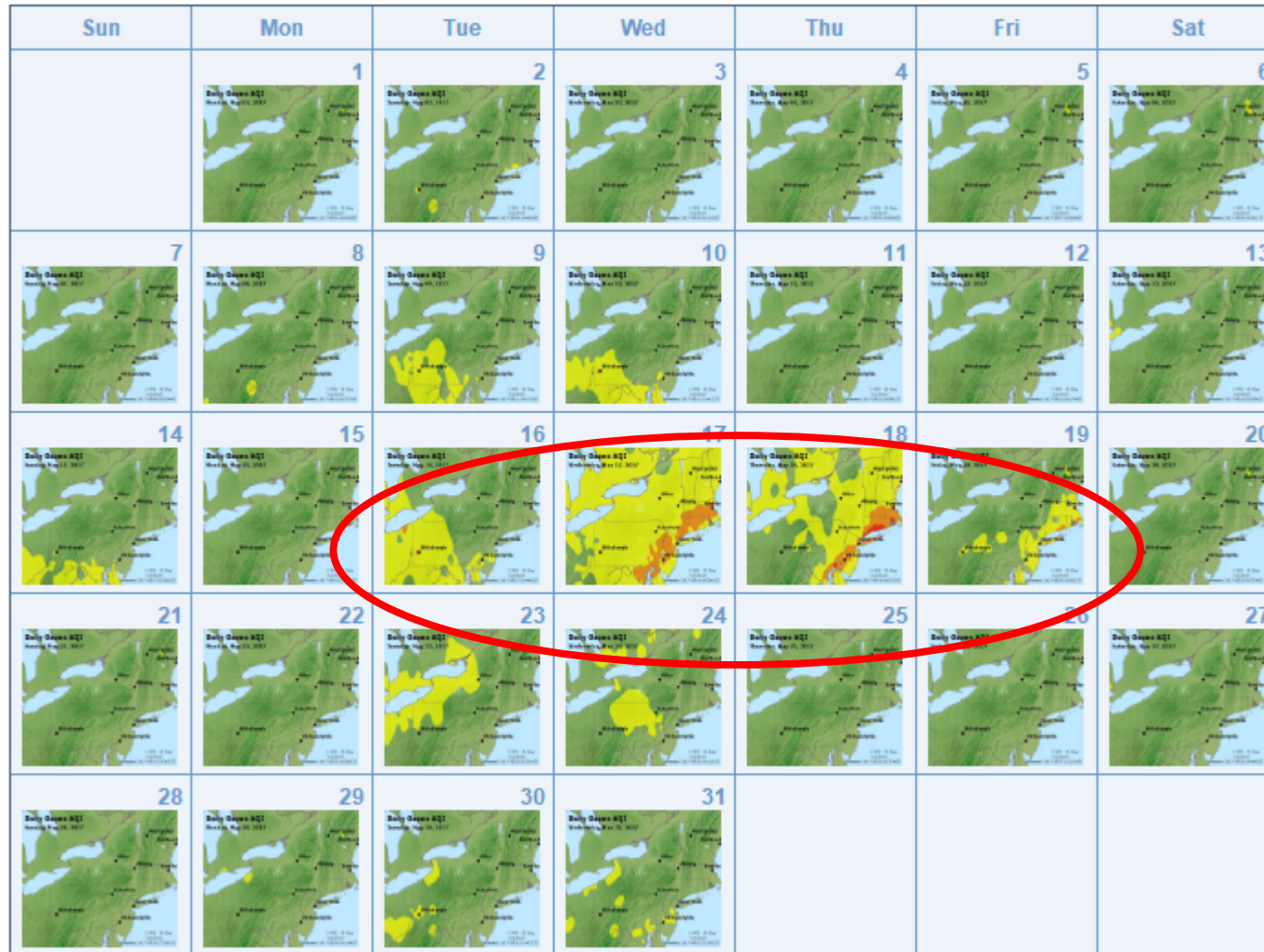
- 2011 NEI (**National Emissions Inventory**) emission data
- available for the contiguous 48 state of the **United States**, **southern Canada** and **northern Mexico**
- Grid spacing: 4km
- NEI (**Hourly emissions**) **different to edgar emis**  
**1° × 1°** )
- Background : Gocart
- Fire emission: Wildfire Automated Biomass Burning



Algorithm (WF\_ABBA)

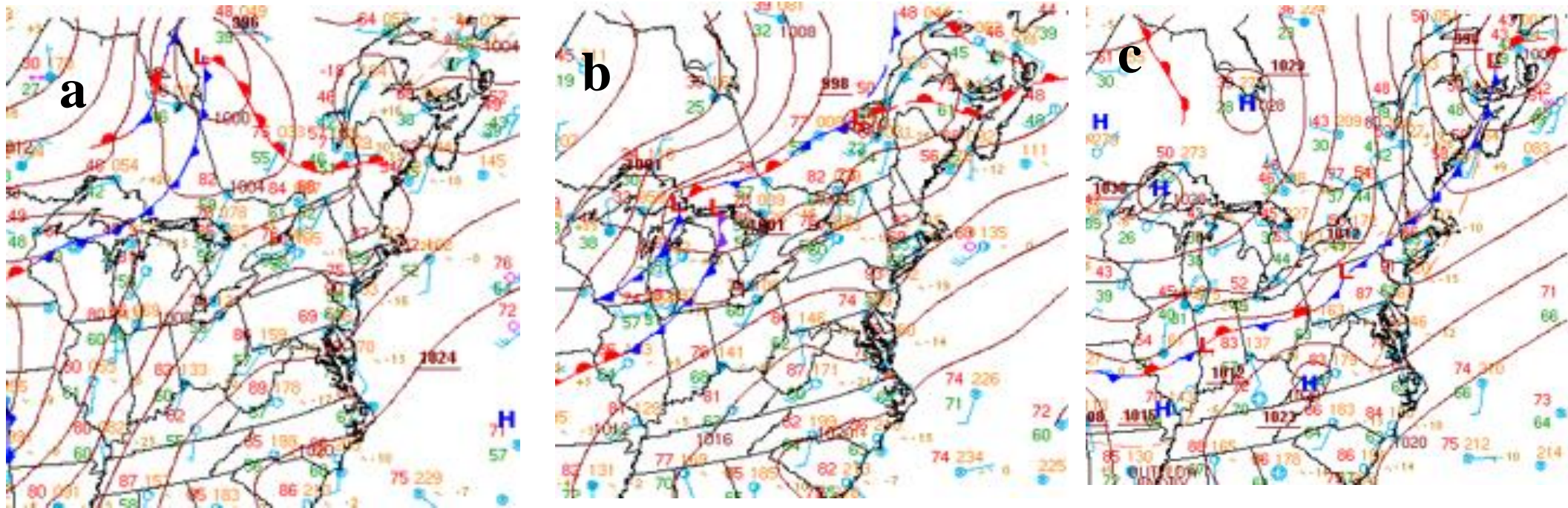


# Results and discussion



**Fig.2 Monthly overview of ozone AQI over New York-Pennsylvania-New Jersey in May 2017 (data access: Environmental Protection Agency, US) .**

# Results and discussion

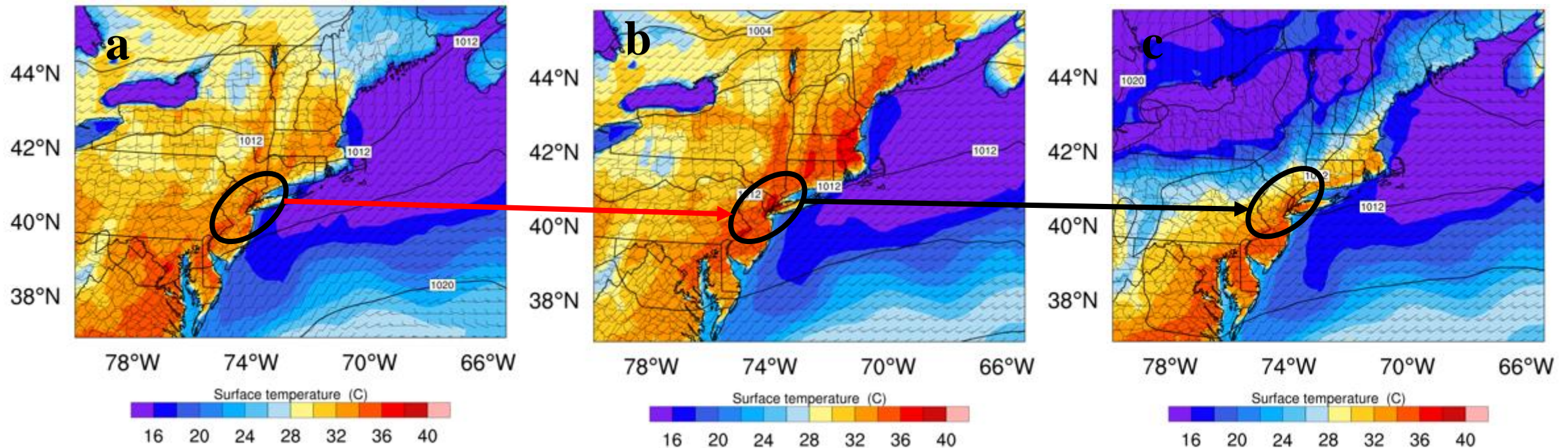


**Fig. 3** Surface weather chart at 1400 LST on May 17-19 2017 (from NOAA North American analysis).

Controlled by the high pressure system and influenced by winds from ocean during the heat wave.



# WRF/Chem-predicted $T_2$



**Fig.4 Predicted  $T_2$  at 14 EST on May (a) 17, (b) 18, and (c) 19, 2017.**

Surface temperature exceeded 36°C on May 18 in New York, which is consistent with the area of high ozone concentrations.<sub>1</sub>



# Evaluations of WRF/Chem-predicted O<sub>3</sub>

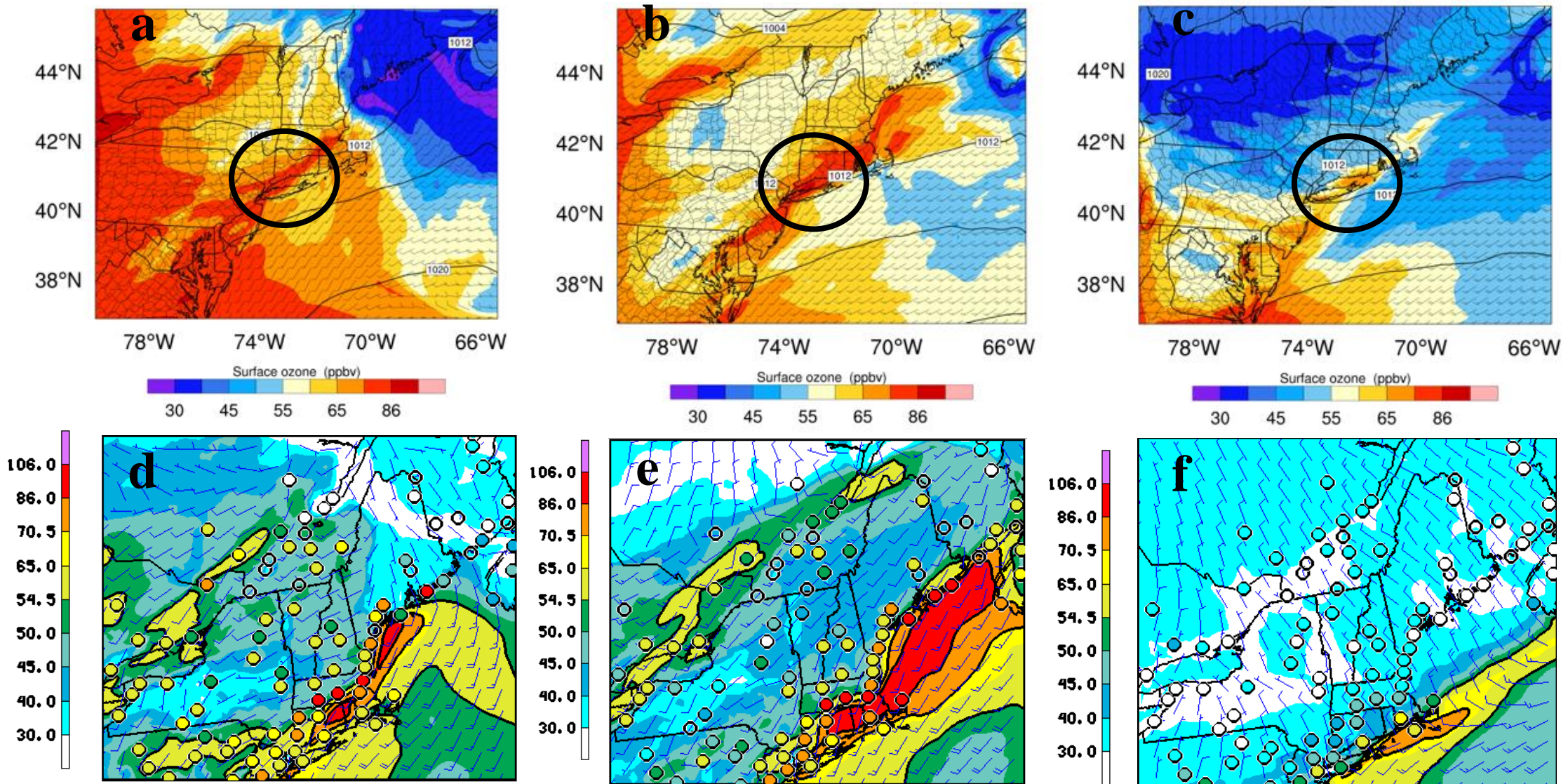
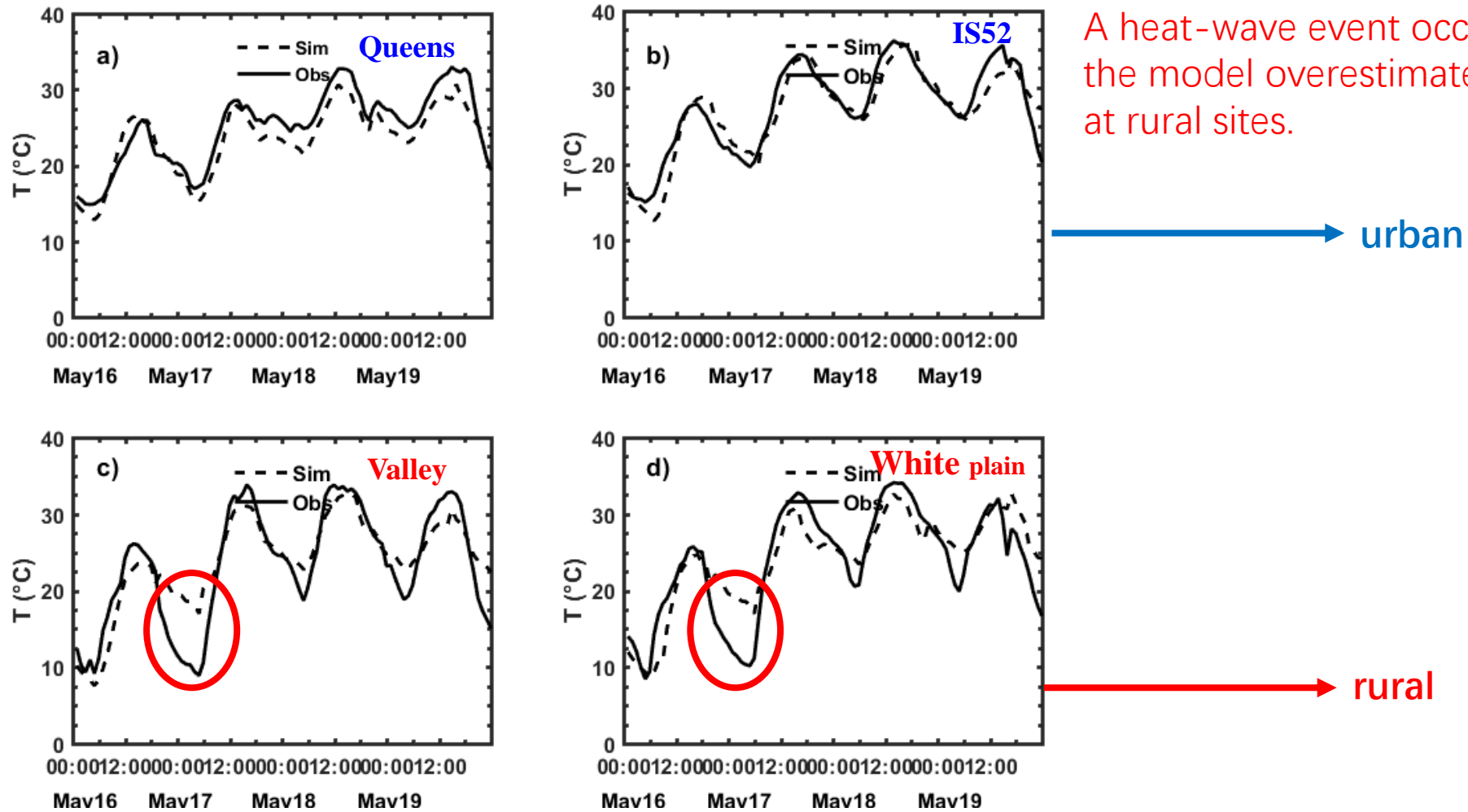


Figure 5. Comparisons of WRF/Chem simulated surface O<sub>3</sub> with the NOAA NMMB-CMAQ products and AirNow observational data on May 17-19, 2017 (a-c: WRF/Chem; d-f: NMMB-CMAQ; dotted points: AirNow)

# WRF/Chem simulated T<sub>2</sub>



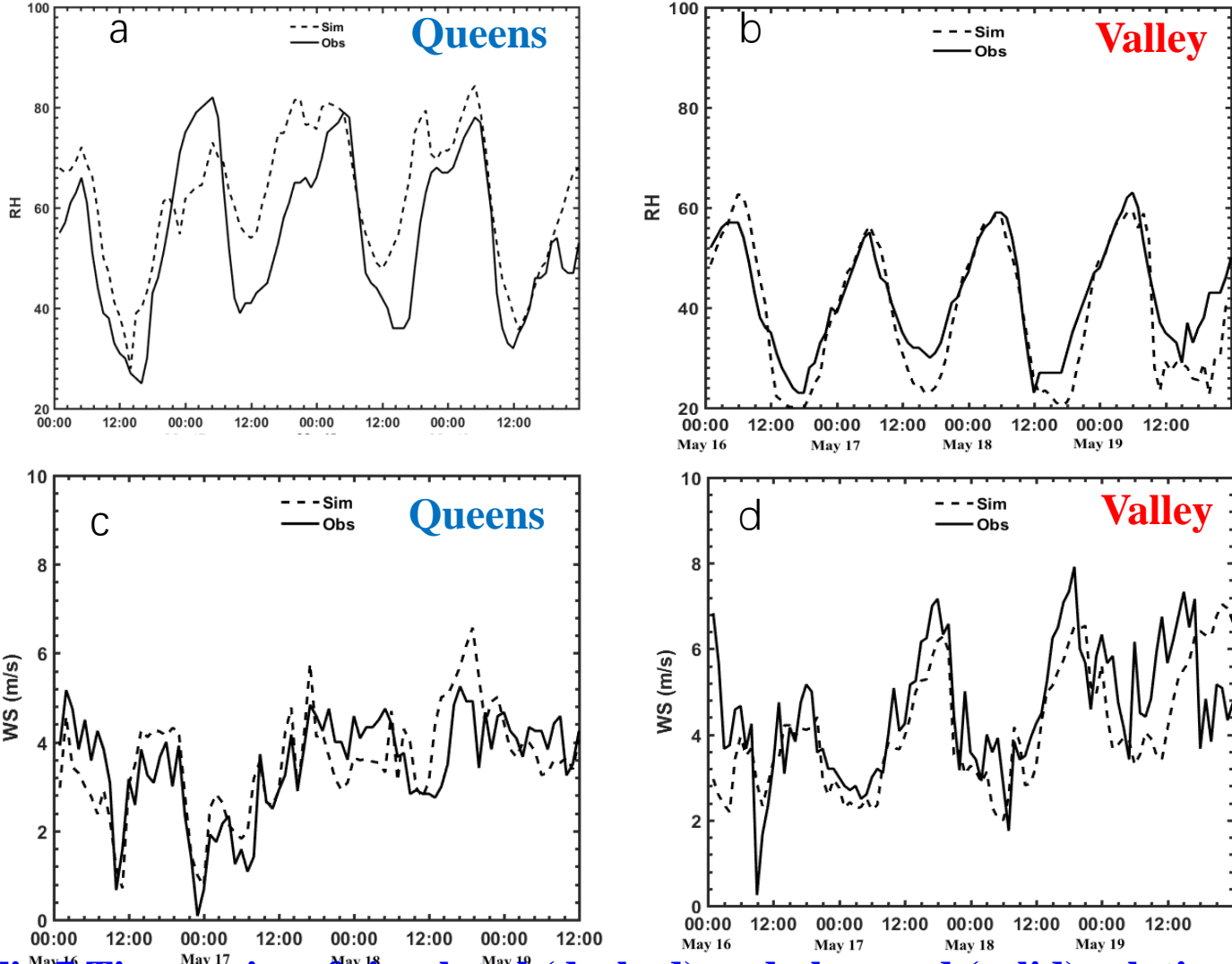
A heat-wave event occurred on May17. and the model overestimates the nighttime minimal at rural sites.

urban

rural

Fig.6 Time series of simulated (dashed) and observed (solid) surface temperature(°C) at a) Queens, b) IS52, c)Valley, d) White plain.

# WRF/Chem simulated RH and WS



The RH was increased greatly and weak-moderate levels wind speeds at urban sites during heat wave event.

Fig.7 Time series of simulated (dashed) and observed (solid) relative humidity at a) Queens, b) Valley and wind speed c)Queens, d) Valley.

# Statistical evaluations of T<sub>2</sub>, RH, and WS

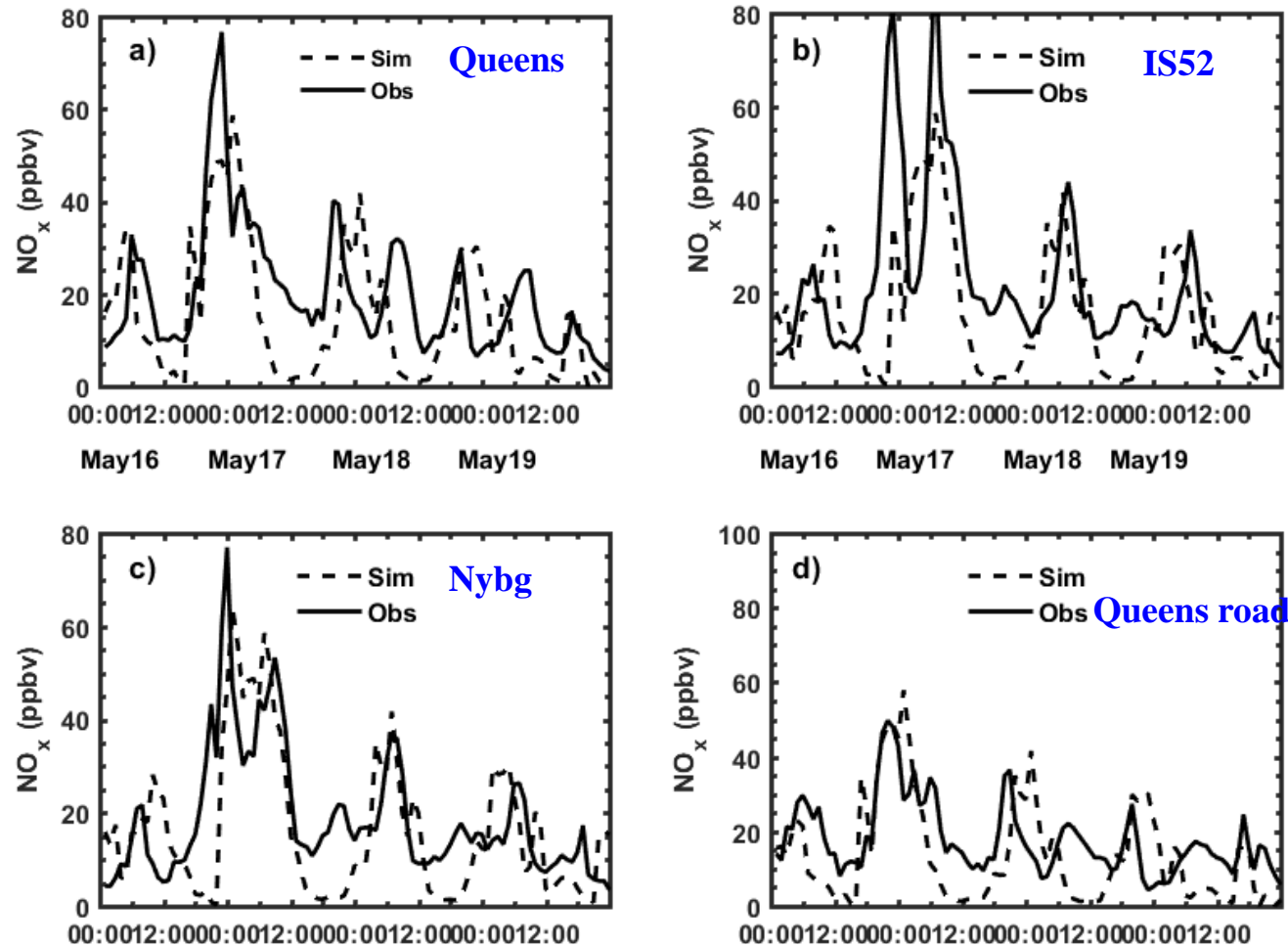
Tab 2. The correlation coefficient, root-mean-square and mean bias errors of measured and predicted at New York (p<0.0001)

	R	RMSE	MB
T(Queens)	0.94	2.22	-1.42
T(IS52)	0.94	2.22	-1.42
T(valley)	0.88	3.64	0.56
T(white plains)	0.86	2.2	-1.42
RH(Queens)	0.81	11.8	7.5
RH(valley)	0.93	6.1	-2.9
WS(Queens)	0.76	0.82	0.05
WS(valley)	0.66	1.3	-0.5

Over-predictions in urban areas  
under-predictions in rural areas.



# Evaluation of predicted NO<sub>x</sub>



**Fig.8** Time series of simulated (dashed) and observed (solid) surface NO<sub>x</sub> (ppbv) at a) Queens, b) IS52, c) Nybg, and d) Queens road



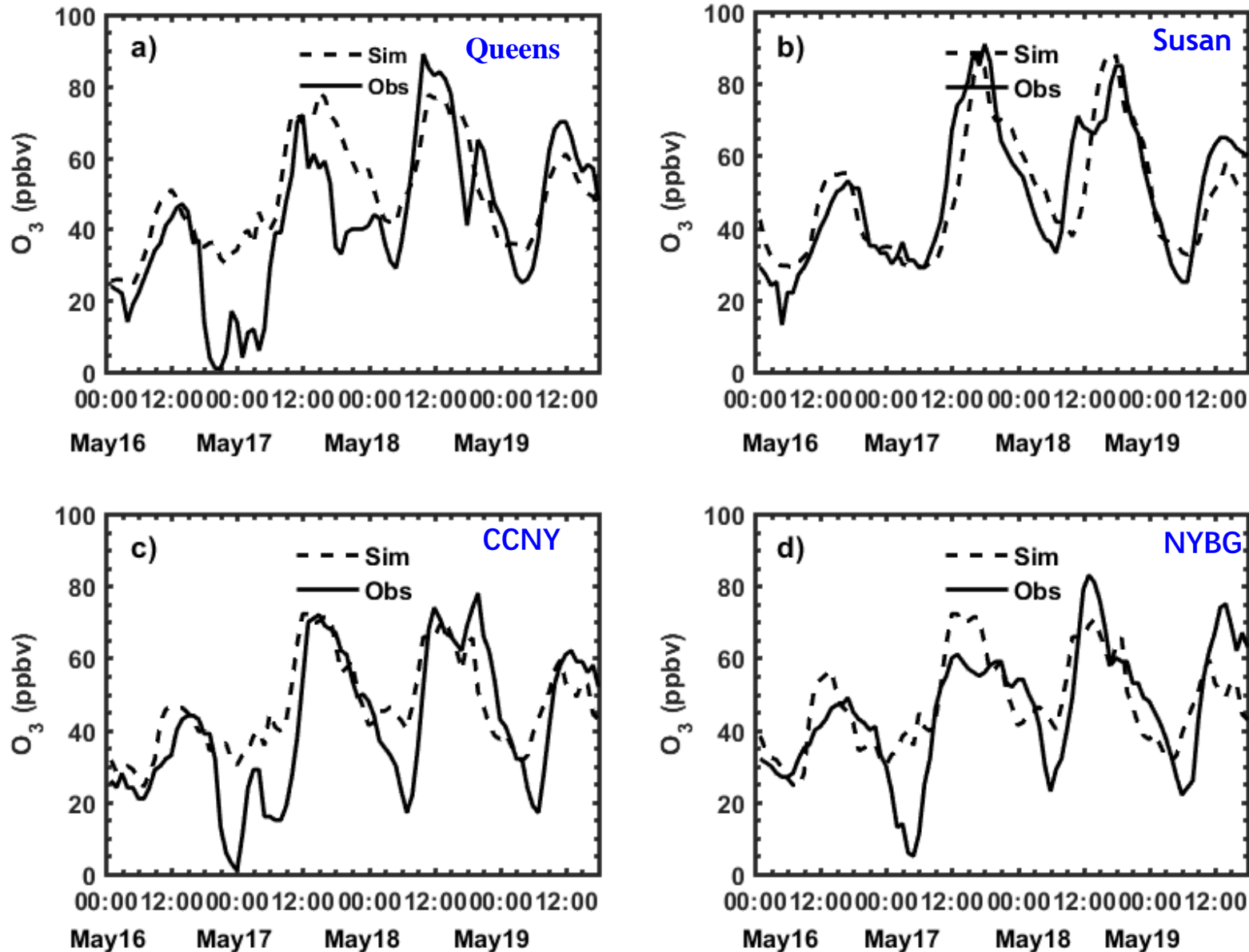
# Statistical evaluations of NO<sub>x</sub>

Tab 3. The correlation coefficient, root-mean-square and mean bias errors of measured and predicted at New York (p<0.0001)

	R	RMSE	MB
NO <sub>x</sub> (QUEENS)	0.57	13.78	-4.83
NO <sub>x</sub> (IS52)	0.5	20.27	-8.47
NO <sub>x</sub> (nybg)	0.64	15.29	-3.54
NO <sub>x</sub> (queens road)	0.55	13.98	-4.83

Under-predicted NO<sub>x</sub> !

# A comparison of simulated O<sub>3</sub> with observations



**Fig.9** Time series of simulated (dashed) and observed (solid) surface O<sub>3</sub> at a) Queens, b) Susan, c) CCNY, and d) NYBG.

WRF/Chem captures the general shape of the diurnal cycle of ozone with minima in the early morning and maxima in the afternoon

# A comparison of simulated O<sub>3</sub> with obs (cont.)

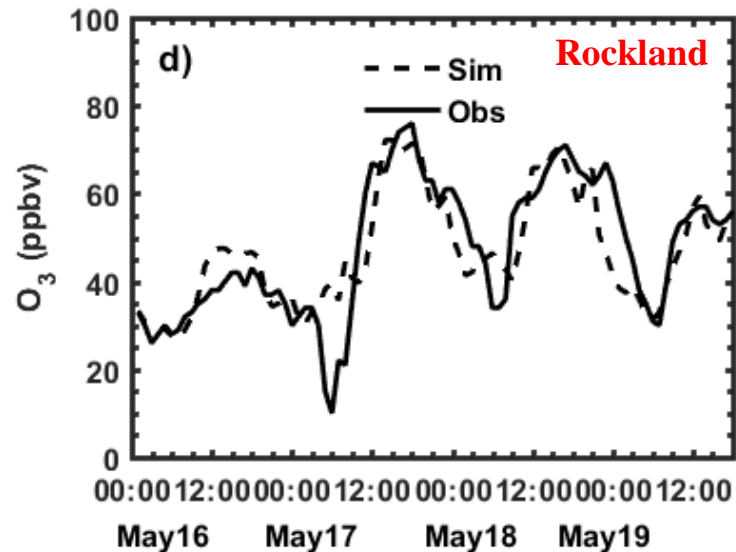
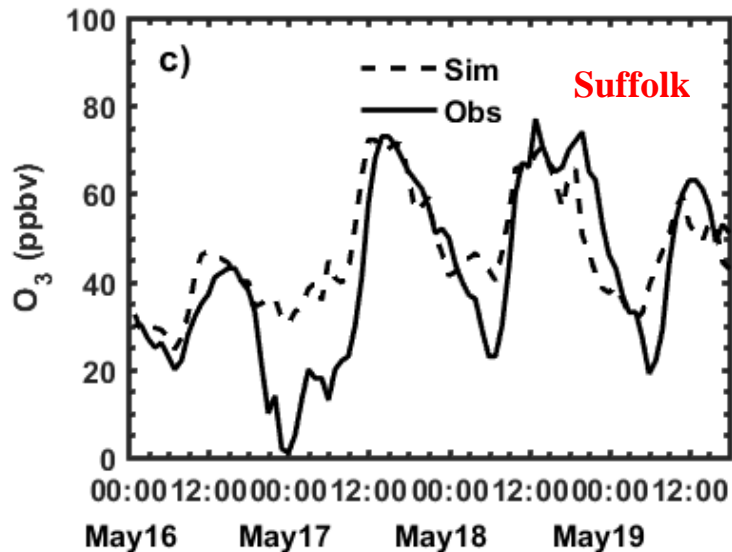
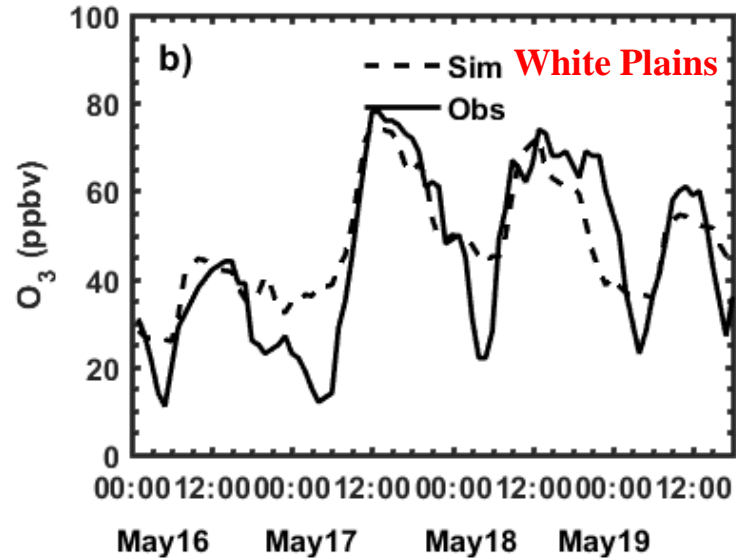
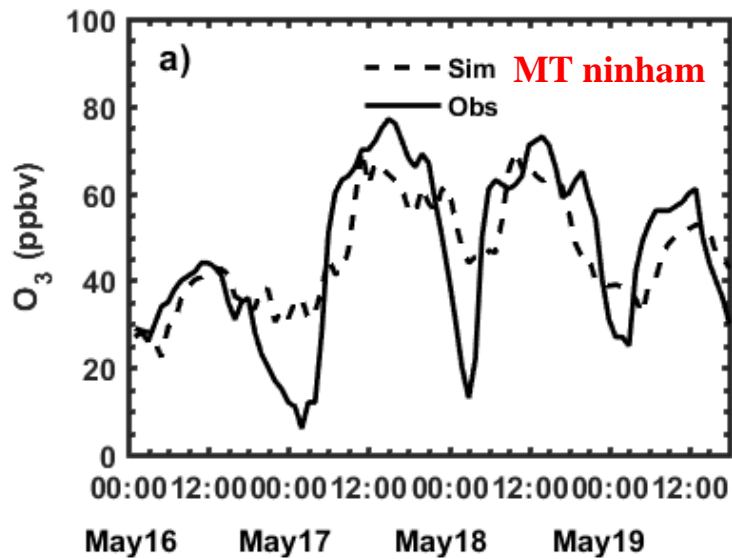


Fig.10 Time series of simulated (dashed) and observed (solid) surface O<sub>3</sub> at a) MT Ninham, b) White Plains, c) Suffolk, and d) Rockland.

# A comparison of simulated O<sub>3</sub> with obs (cont.)

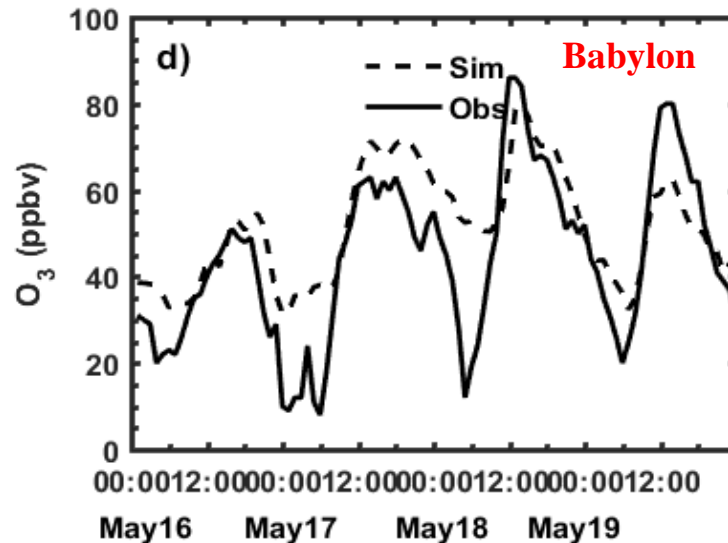
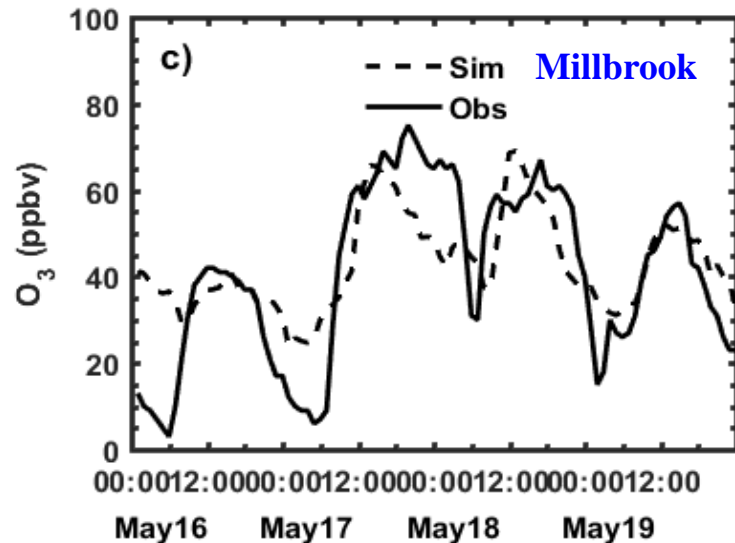
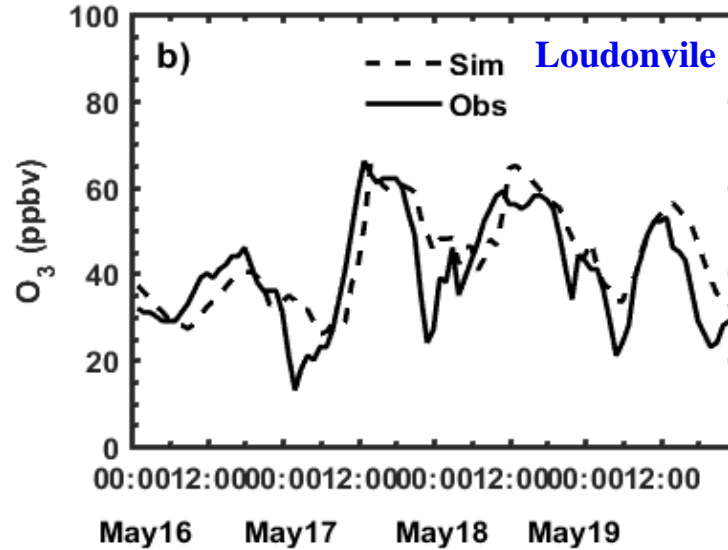
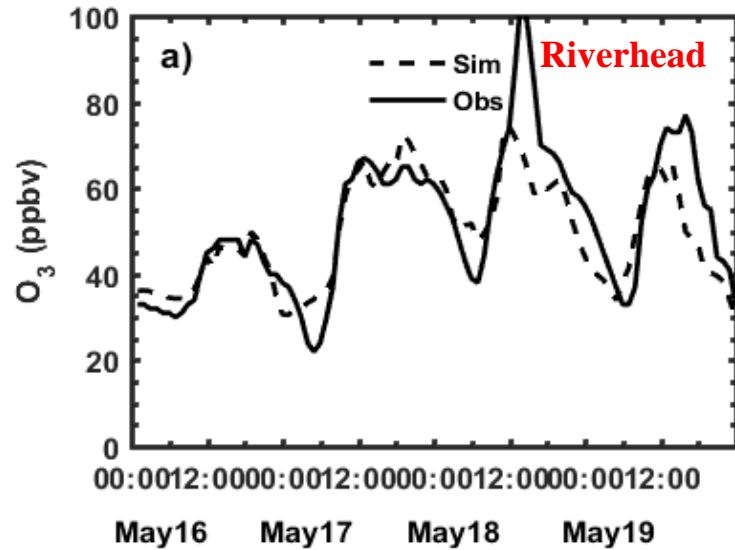


Fig.11 Time series of simulated (dashed) and observed (solid) O<sub>3</sub> at a) Riverhead, b) Loudonville, c) Millbrook, and d) Babylon.

The model over-predicted at nighttime and captured the ozone peak quite well.

# Statistical evaluations of O<sub>3</sub> predictions

Tab 4. The correlation coefficient, root-mean-square and mean bias errors of measured and predicted at New York (p<0.0001)

	R	RMSE	MB
Queens	0.78	14.8	7.23
Susan	0.86	9.5	-0.54
Ccny	0.78	13.2	5.35
NYBG	0.7	12	2.06
MT Ninham	0.82	11.56	0.6
White plains	0.86	10.57	2.46
Suffolk	0.81	-7.23	-0.72
Rockland	0.83	12.27	-0.61
Riverhead	0.84	9,43	-2.32
Loudonvile	0.77	8.6	2.9
Millbrook	0.77	13.6	2.1
babylon	0.81	8.17	-2.32

# Evaluations of daily 8-hr max O<sub>3</sub> predictions

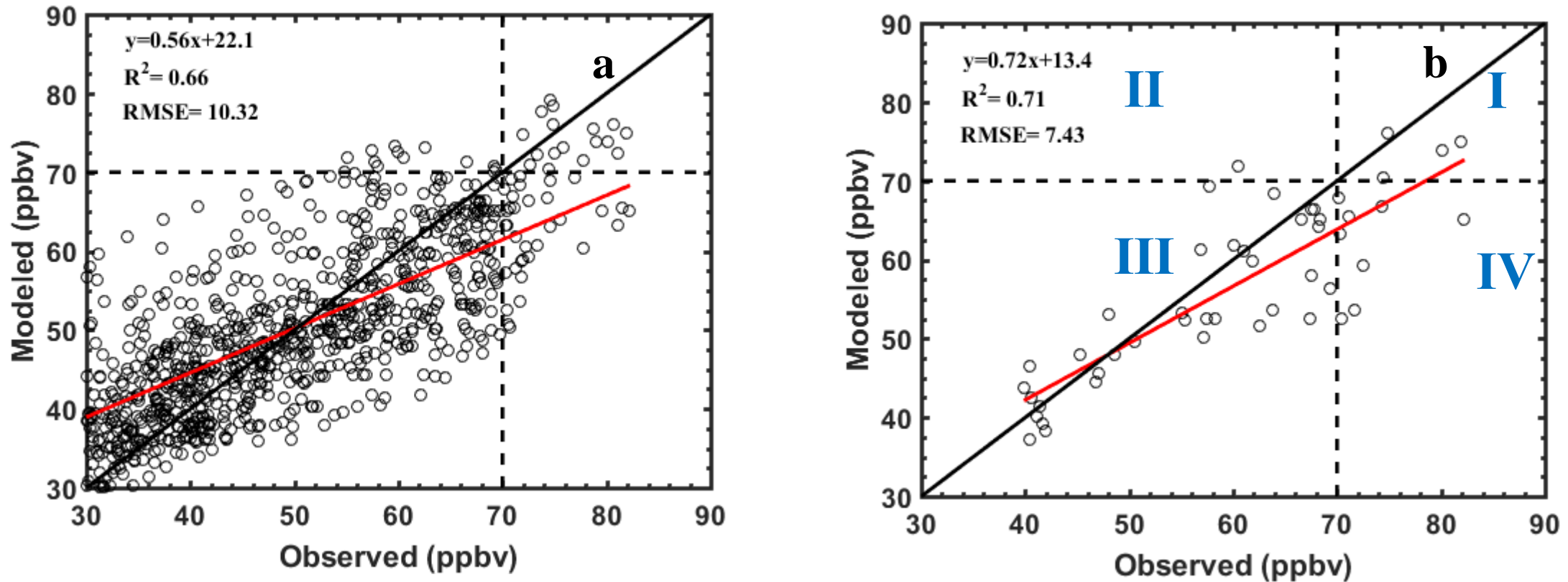


Figure 12. Scatter plot of the simulated vs. observed (a) 8-h average and (b) daily 8-hr maxima O<sub>3</sub> on May 17-19 2017 (Note: exceedance thresholds: 70 ppbv)

Over-predicted at low concentration (<50.0 ppbv) but under-predicted at high concentrations (> 50.0 ppbv)

# Evaluations of daily 8-hr max O<sub>3</sub> predictions

- ◆ I : a forecast 8 h exceedance (>70 ppbv) that did occur
- ◆ II : a forecast 8 h exceedance that did not occur
- ◆ III : a forecast 8 h nonexceedance that did occur
- ◆ IV : a nonforecast 8 h exceedance that did occur

$$\text{FAR} = \left( \frac{\text{II}}{\text{I} + \text{II}} \right) \cdot 100\% = 2\% \text{ (False alarm ratio)}$$

$$\text{CSI} = \left( \frac{\text{I}}{\text{I} + \text{II} + \text{IV}} \right) \cdot 100\% = 31\% \text{ (Critical success index)}$$

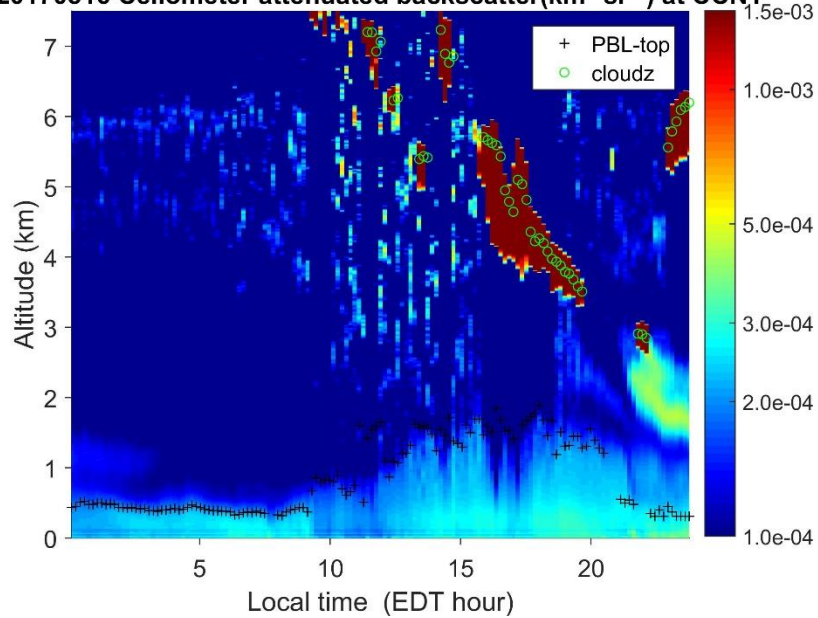
FAR : the percentage of times an exceedance was forecast when none occurred

CSI : how well forecasted and measured exceedances were predicted

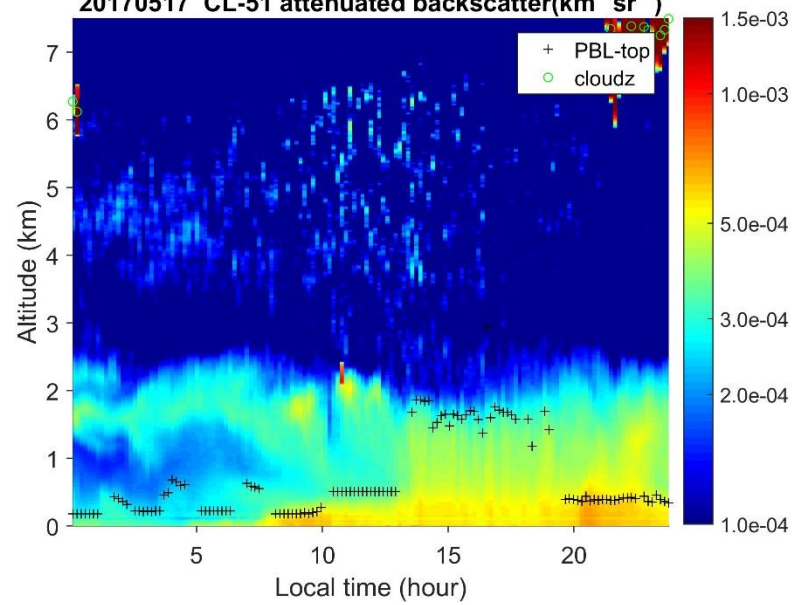


# Results: backscatter Lidar

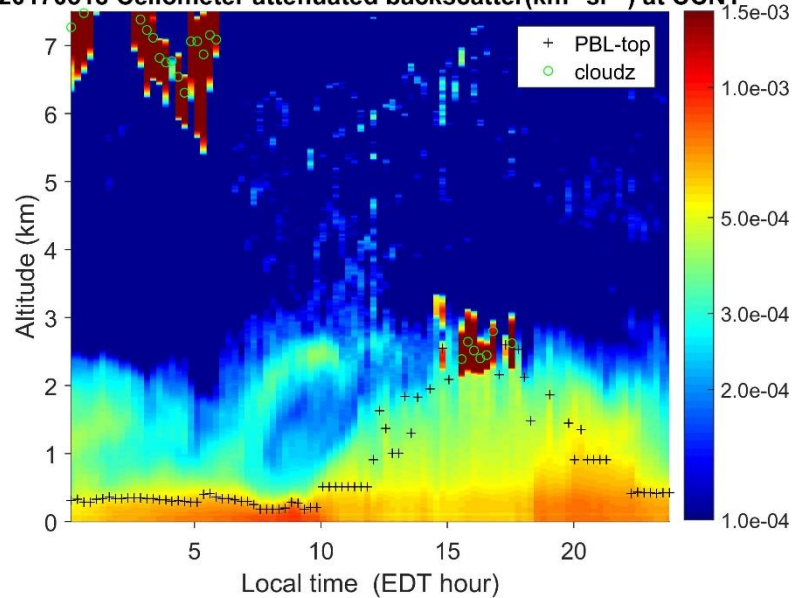
20170516 Ceilometer attenuated backscatter( $\text{km}^{-1}\text{sr}^{-1}$ ) at CCNY



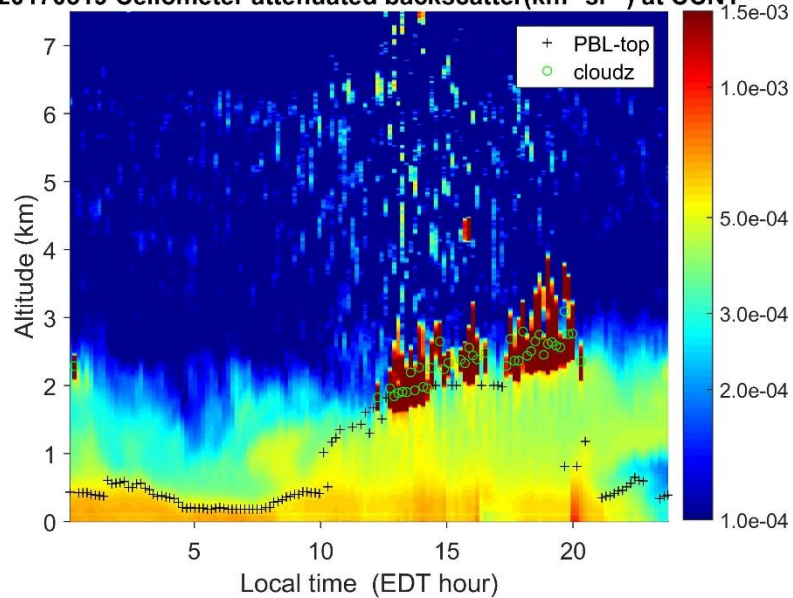
20170517 CL-51 attenuated backscatter( $\text{km}^{-1}\text{sr}^{-1}$ )



20170518 Ceilometer attenuated backscatter( $\text{km}^{-1}\text{sr}^{-1}$ ) at CCNY



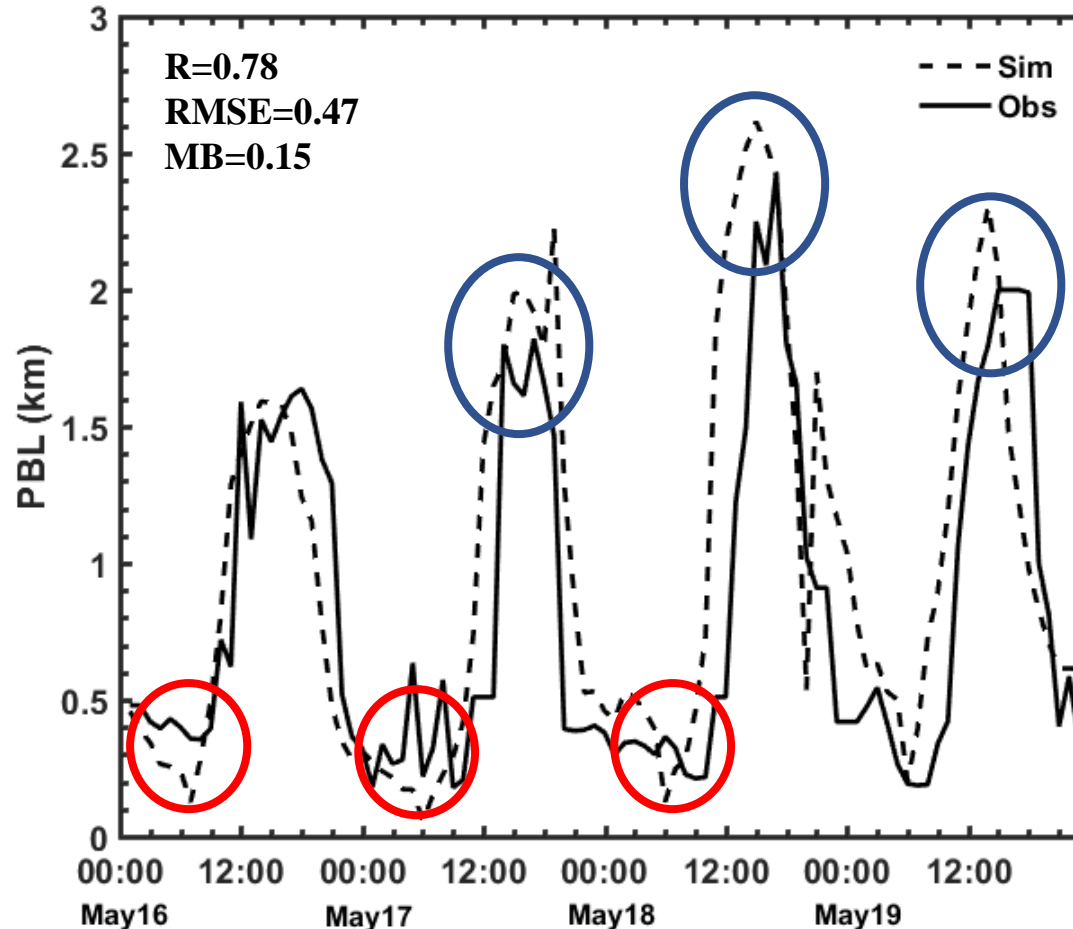
20170519 Ceilometer attenuated backscatter( $\text{km}^{-1}\text{sr}^{-1}$ ) at CCNY



**Fig 13. Spatial and temporal distribution of observed daily mean attenuated backscatter index at CCNY during May 16-19 2017 (Black cross: PBL height)**



# Results: planetary boundary layer



Underestimated at nighttime (cause ozone over-predictions)

Overestimated at daytime (under-predictions of ozone)

Fig.14 Time series of simulated (dashed) and observed (solid) planetary boundary layer height (km) at CCNY

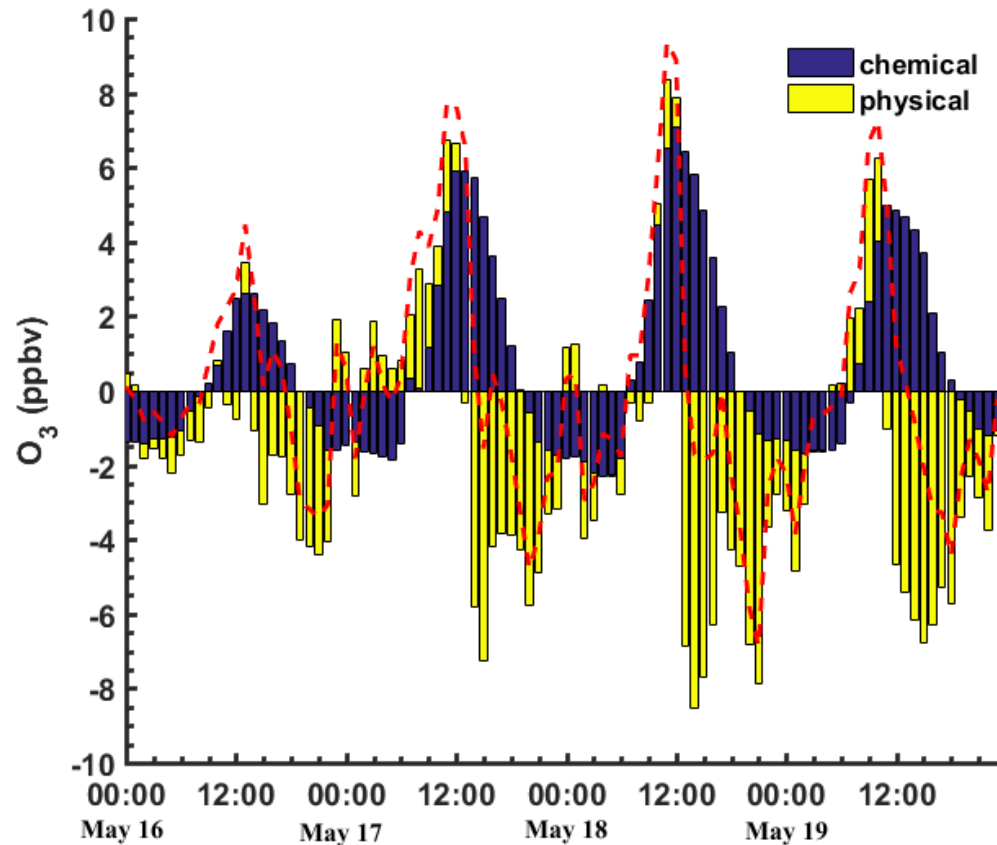
# Results: Statistical surface tem and ozone

Tab 5 Comparisons of daily 8-hr max and mean value of ozone and temperature at 12 stations

	O <sub>3</sub> (mean)	O <sub>3</sub> (max)	T(max)
16	31.7 (26-39)	44	26.9
17	45.7 (38-56)	66	31.2
18	56.7 (52-64)	73	34.4
19	46.5 (42-53)	63	34.1
16	31.8 (26-37)	43	25.9
17	46.1 (41-50)	59	33.3
18	54.3 (48-61)	66	33.9
19	41.6 (36-47)	53	32.5

Increase in O<sub>3</sub> in urban areas is higher than that in rural areas

# Process analyses of O<sub>3</sub> change



The chemical production is increased gradually

Chemical contribution  
16<sup>th</sup>: 13.7 ppbv  
17<sup>th</sup>: 34.1 ppbv  
18<sup>th</sup>: 39 ppbv  
19<sup>th</sup>: 29.8 ppbv

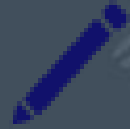
Fig 15 O<sub>3</sub> change due to chemical reactions and physical transport in the surface layer at 12 sites on May 16-19, 2017 (Red dashed line: net change)

# Summary

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A high-resolution model WRF/Chem was **successful** to simulate the meteorological fields, NO<sub>x</sub>, and O<sub>3</sub> during a heat wave driven ozone exceedance event in New York and surrounding areas.



The daytime underestimation of O<sub>3</sub> is mainly attributed to the **over-predicted boundary layer height** and **underestimated ozone precursors (e.g., No<sub>x</sub>)**. The overprediction of nighttime O<sub>3</sub> is attributed to a **high vertical mixing coefficient**, **underestimated boundary layer** in the model.



The process analyses show the **chemical production increased gradually** and was the biggest contributor (i.e., 39 ppbv ) to the ozone exceedance event during the heat wave related event.

# Future work

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- ❖ To develop a manuscript.
- ❖ To investigate the impact of long-range transport on the wildfire associated severe ozone pollution episode.
- ❖ To compare high resolution(1.3km) WRF/Chem simulations with the NOAA NMMB-CMAQ products (12km) for evaluating the impact of high resolution simulations on air quality forecasting, especially for the sea-breeze related air pollution events.





Thanks