An Assessment of Community Multiscale Air Quality Model Performance of Oxides of Nitrogen, Reactive Oxidized Nitrogen, and Ozone over Rural and Urban New York State During Summer 2015

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Introduction

This study examined how accurately two Community Multiscale Air Quality (CMAQ) model versions predicted concentrations of oxides of nitrogen ([NO_x]), reactive oxidized nitrogen ([NO_y]), and ozone ([O_3]) over rural and urban New York State (NYS). To assess model performance of those species, the CMAQ model-predicted versus observed ozone production efficiency (OPE) for August 2015 was compared for rural and urban NYS.

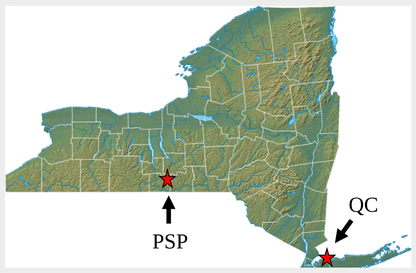
Research focused on two questions:

1) What is a typical OPE in rural and urban NYS, and how well does the CMAQ model-predicted OPE reflect the observed OPE?

2) What meteorological factors led to similarities or discrepancies in predicted versus observed OPE during August 2015?

Methods

- Time period of interest was 1-28 August 2015
- Model platforms used were 1) CMAQ Version 4.6 (v4.6) and 2) CMAQ Version 5.0.2 (v5.0.2)
- NO_x, NO_y, and O_3 model predictions and measurements for 1) Pinnacle State Park (PSP, rural site) in Addison, New York (NY), and 2) Queens College (QC, urban site) in Flushing, NY were used



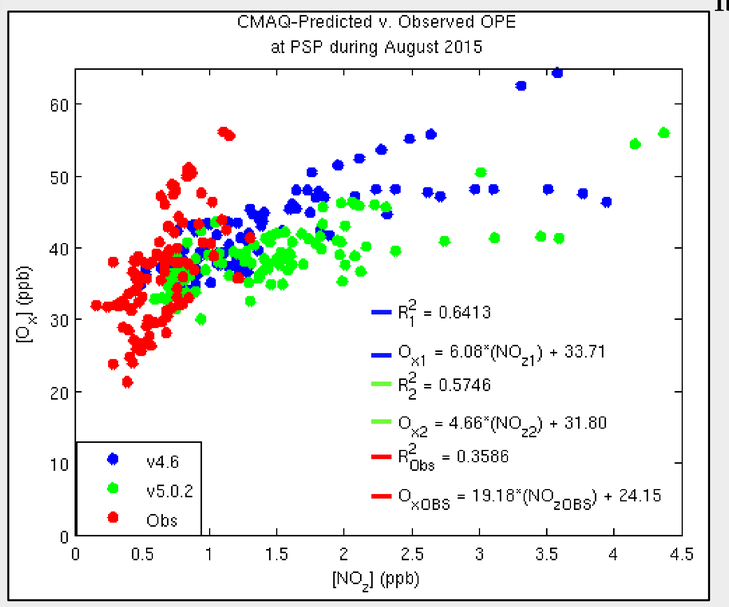
- OPE was calculated in the following way:
  - OPE = ΔO_x / ΔNO_z, where:
    - O_x = O_3 + nitrogen dioxide (NO_2)
    - NO_z = NO_y - NO_x
- Three data filters were applied to analyze OPE:
  - Photo-chemically productive hours (11 a.m. – 4 p.m. Eastern Standard Time (EST))
  - Periods where little cloud cover was predicted by the model (Total Cloud Fraction < 0.5)
  - Periods where no precipitation was observed or predicted
- Two meteorological factors were examined to explore similarities and differences in forecasted versus observed OPE:

1) Dry deposition at PSP

2) Planetary boundary layer height (PBLH) at QC

Results – Ozone Production Efficiency

1a)



1b)

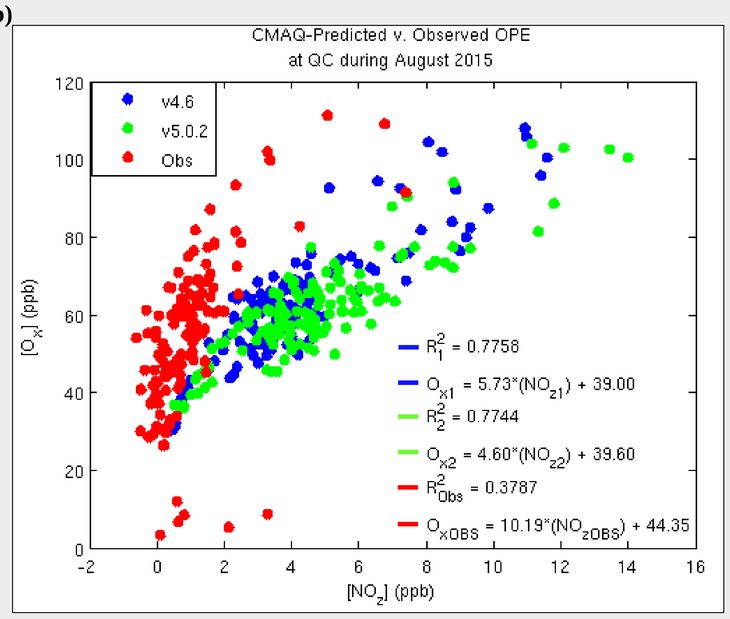
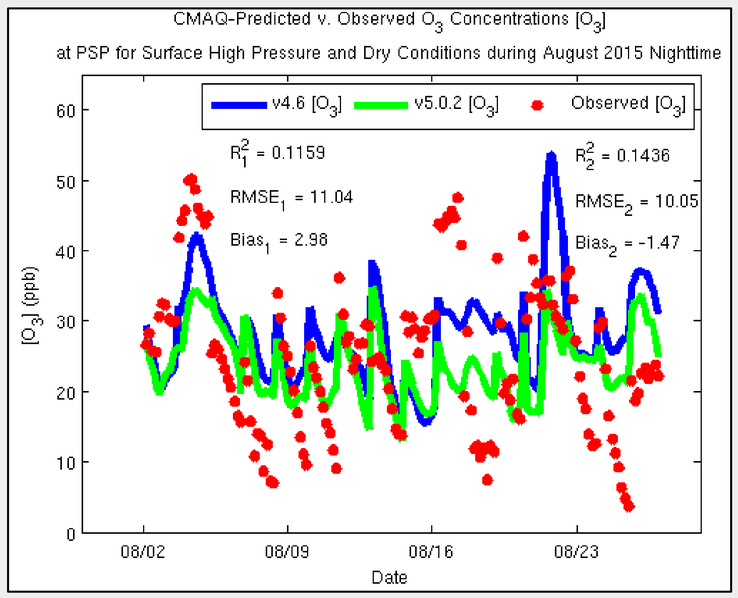


Figure 1. a) CMAQ-predicted versus observed OPE at PSP from 1-28 August 2015. Statistical variables and slope-intercept equations with subscripts of 1, 2, or OBS correspond to the results for CMAQ v4.6 (blue dots), CMAQ v5.0.2 (green dots), and observations (red dots), respectively. **b)** Same as 1a), except it is plotted for QC.

Results – Nighttime Ozone (PSP) and Boundary Layer Heights (QC)

2)



3)

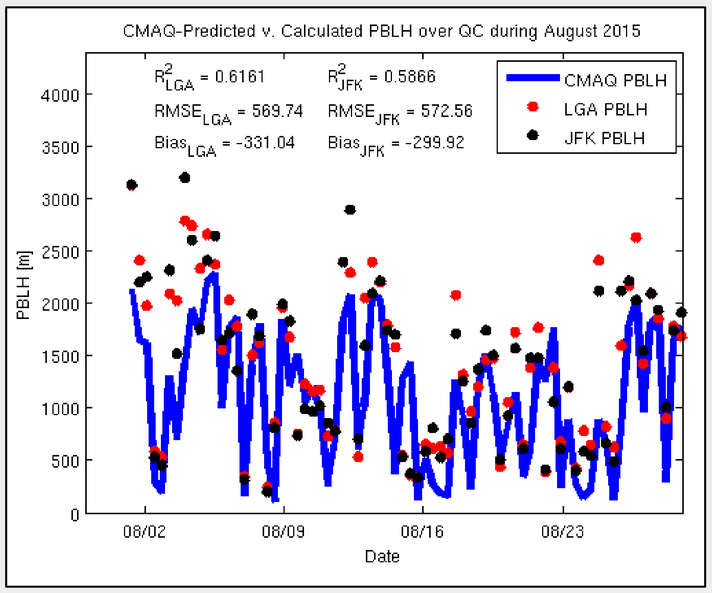


Figure 2. Time series of [O_3] concentrations at PSP during August 2015 nighttime hours when dry deposition of O_3 likely occurred. Statistical variables with a subscript of 1 correspond to the relationship between CMAQ v4.6 results (blue line) and observations (red dots). Statistical variables with a subscript of 2 correspond to the relationship between CMAQ v5.0.2 results (green line) and observations.

Figure 3. CMAQ-predicted versus calculated PBLH over QC during August 2015. Statistical variables with the subscript "LGA" correspond to the relationship between the CMAQ-predicted PBLH (blue line) and the calculated PBLH at LaGuardia Airport (red dots). Statistical variables with the subscript "JFK" correspond to the relationship between the CMAQ-predicted PBLH and the calculated PBLH at John F. Kennedy International Airport (black dots).

Conclusions

- Model-predicted and observed OPE were in better agreement at QC than at PSP
  - We hypothesize that this result is due to better agreement at QC in the individual chemical species (e.g. NO_x, NO_y, and O_3), which, in turn, is partially due to good representation of the PBLH
- Model-predicted and observed OPE were in poor agreement at PSP
  - Partitioning of ΔO_x and ΔNO_z into components is likely needed
    - Gas-phase chemistry
    - Dry deposition
  - Difference in measurement height (5 meters (m)) and the height of the middle of the lowest level in CMAQ (20 m) could have had an impact
- CMAQ v4.6-predicted and CMAQ v5.0.2-predicted OPE were very similar at both sites

Future and Ongoing Work

- Extend OPE analysis to include summer 2016 (June-September)
  - Utilize a more complete dataset of NO_y observations from a field intensive at both sites to compare to CMAQ model output
- Study O_3 production rate (P_{O3}) at PSP and QC using both CMAQ model output and observations
  - Assess the role of NO_x and volatile organic compounds (VOCs) in O_3 formation
  - Use different indicator ratios of O_3 sensitivity – such as VOC:NO_x and formaldehyde (HCHO):NO_z – to study whether O_3 forms in VOC-limited or NO_x-limited conditions
    - Assess potential regulatory impact
- Explore more completely the modeled and observed dependence of OPE on NO_x
  - PSP especially straddles the NO_x regime where values of P_{O3} and OPE are rapidly changing

Acknowledgements

- Matthew Ninneman and Dr. James Schwab acknowledge support from NYSERDA (New York State Energy Research and Development Authority) contract numbers 48971 and 59807.
- We are grateful to site operators John Spicer at PSP (ASRC) and Mike Christopherson at QC (NYS DEC) for their contributions. We also acknowledge New York State Department of Environmental Conservation for logistical and in-kind support at both sites.

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