OTC 8-Hour Ozone Modeling Results 2002 Base Case Performance One-Atmosphere Modeling Platform

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Background

- OTC Modeling Committee charge to its members

- NYDEC initiated the SIP modeling platform design

- UMD with support from MDE developed the meteorological fields for 2002 using MM5

- MARAMA and contractor worked with MANEVU states to prepare 2002 base year emission inventory

Multi-P Modeling Centers

- NYSDEC, MDE/UMD, NJDEP/Rutgers ORC, NESCAUM, and VADEQ

- All centers participated in a benchmark of CMAQ and SMOKE models to assess compatibility between different hardware/software platforms

- Benchmark tests revealed good compatibility between the centers within computational constraints of the hardware/software systems

Modeling Domain

36 km
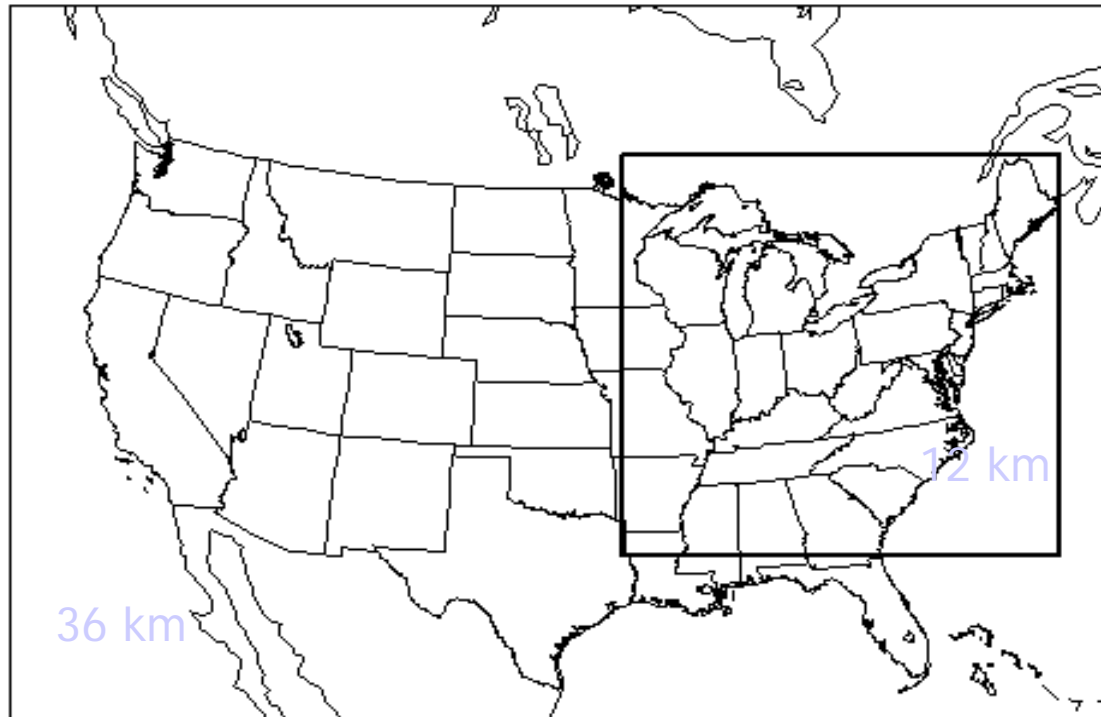
12 km

CMAQ Model Set-up

- Horizontal grid resolution at 36 and 12 km, with 22 levels in the vertical

- Models: CMAQ v4.4, SMOKE v2.1, MM5 v3.6-3

- 2002 Emissions developed through MANE-VU

- to provide BCs for the CMAQ 12 km domain

Ozone Modeling Assessment

- Simulation covers April through October 2002

- Model assessment statistics for O_3, NO, NO_2, CO, SO_2, Isoprene, Ethane, Formaldehyde, and NO_x/TNMOC ratios

- Spatial distribution of daily observed and predicted maximum 8-hour O_3 concentrations at 12 km posted at
ftp://www.dec.state.ny.us/dar/air_research/mku

- Model evaluation statistics for daily maximum 1-hour and 8-hour O_3 posted at
ftp://www.dec.state.ny.us/dar/air_research/kevin

Performance Goals

- Correctly Depict Spatial Patterns (*Failure here would raise doubts of the model's usefulness in simulating future scenarios*)

- Show No Strong Bias (*Consistent over or under-predicting better than random; underpredictions could mean weak model sensitivity to future case reductions*)

- Correctly Render Sea Breeze Effects and Gradients (*Of primary importance in many coastal areas*)

Performance Statistics

1. Coefficient of determination (R^2)
2. Normalized mean error (NME), %
3. Root mean square error (RMSE), ppb
4. Fractional gross error (FE), %
5. Mean absolute gross error (MAGE), ppb
6. Mean normalized gross error (MNGE), %
7. Mean bias (MB), ppb
8. Mean normalized bias (MNB), %
9. Mean fractionalized bias (MFB), %
10. Normalized mean bias (NMB), %

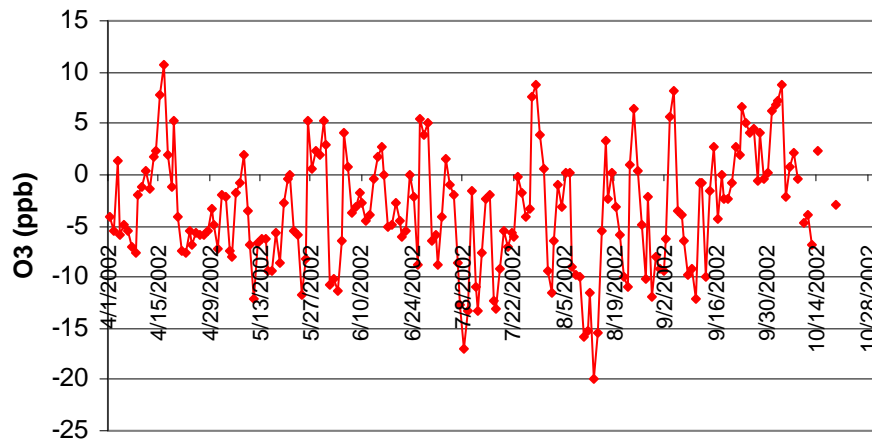# Coefficient of determination (r²) for daily maximum 8-hour O₃

- ● < 0.4
- ● 0.4-0.5
- ● 0.5-0.6
- ● 0.6-0.7
- ● 0.7-0.8
- ● > 0.8
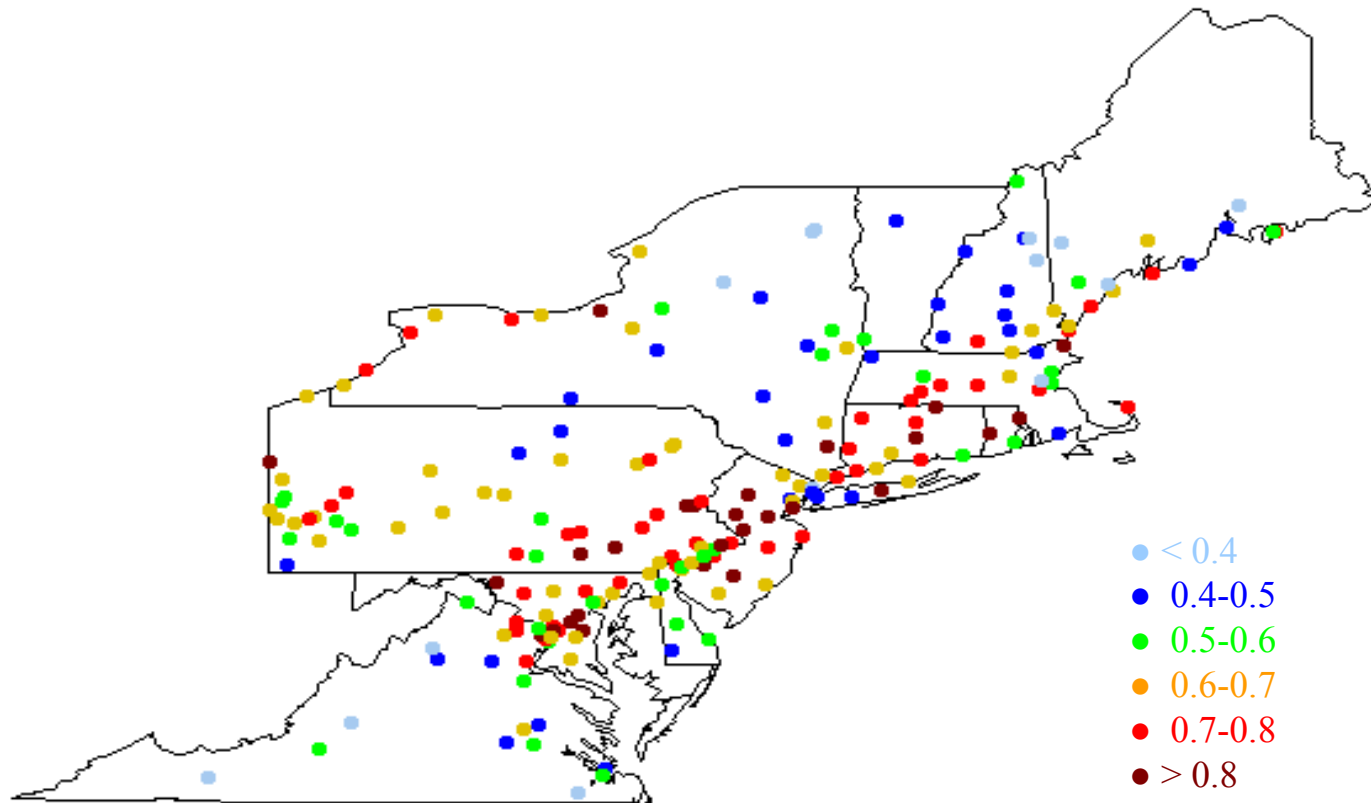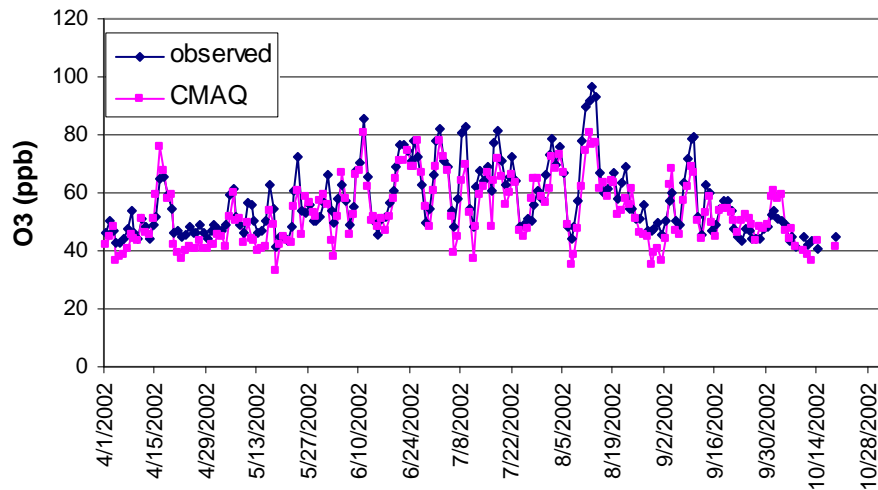
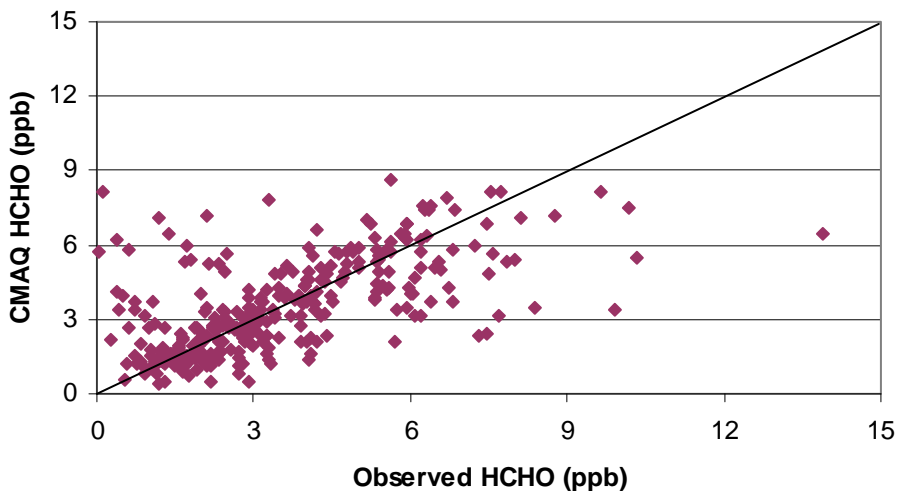Domain-wide average daily maximum 8-hour O_3

Daily average Ethene, June-August
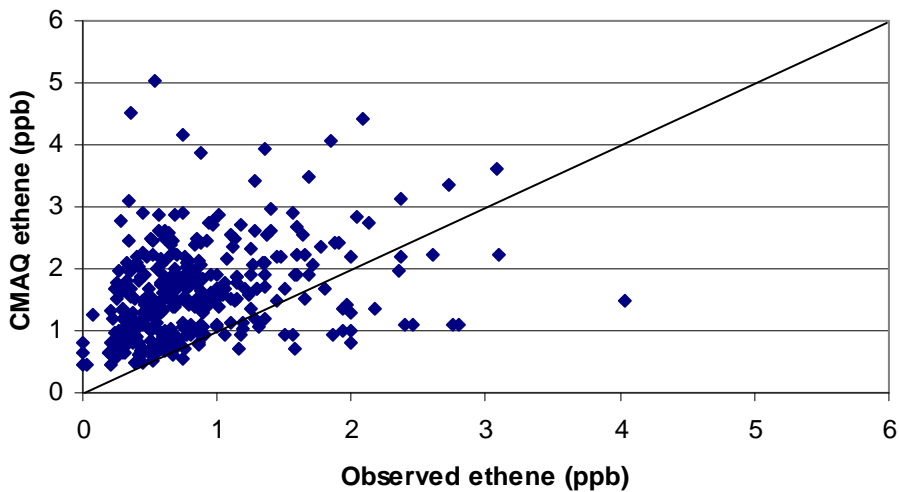
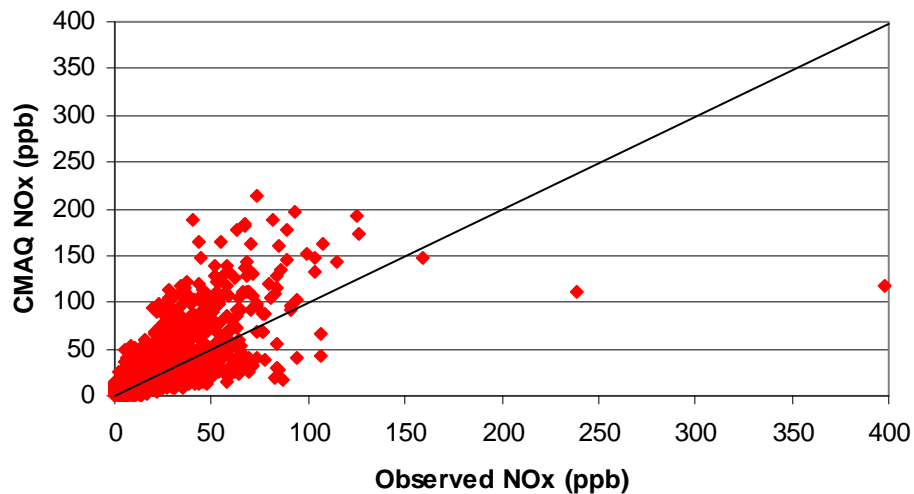Daily average Isoprene, June-August
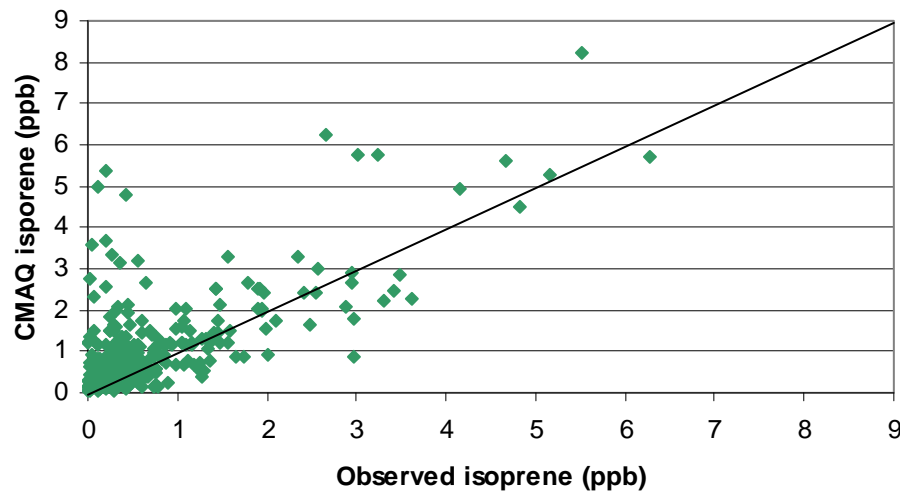
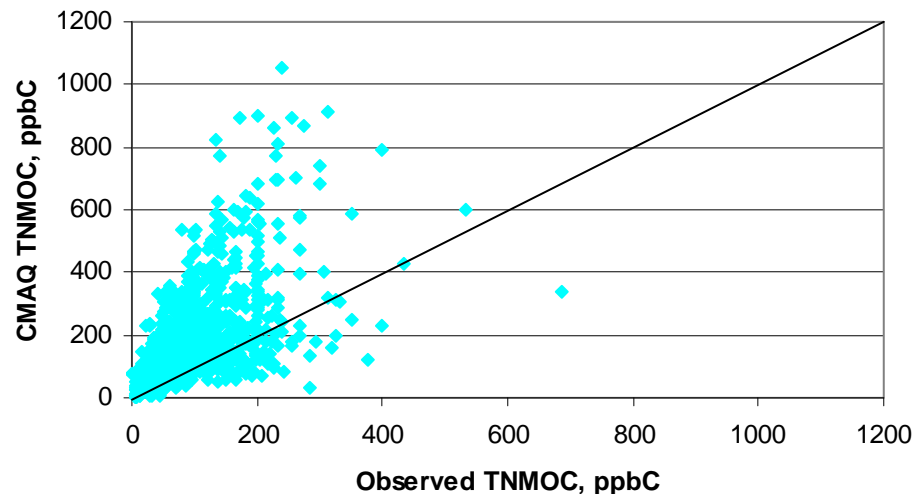Daily average Formaldehyde, June-August

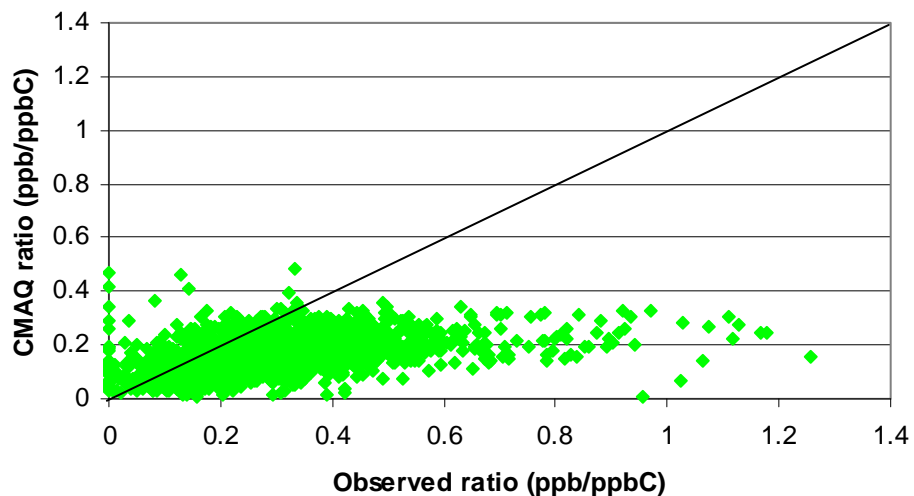Daily average ethene, isoprene, and formaldehyde concentrations

6-9 am NOx, June-August
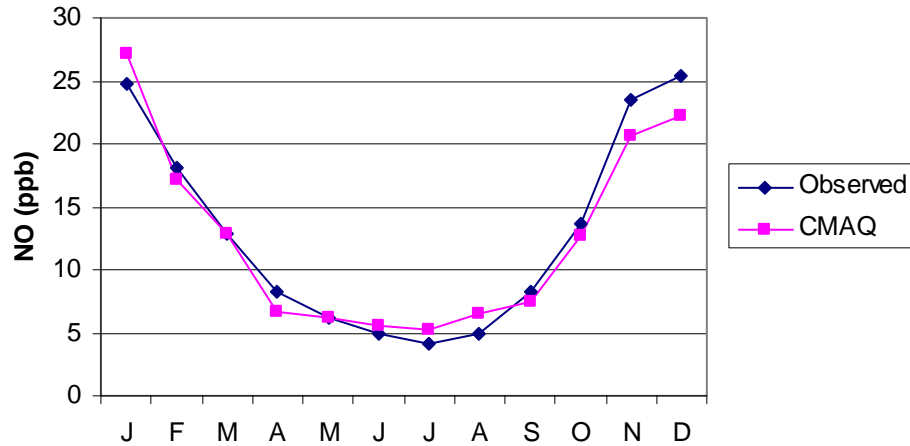
6-9 am TNMOC, June-August
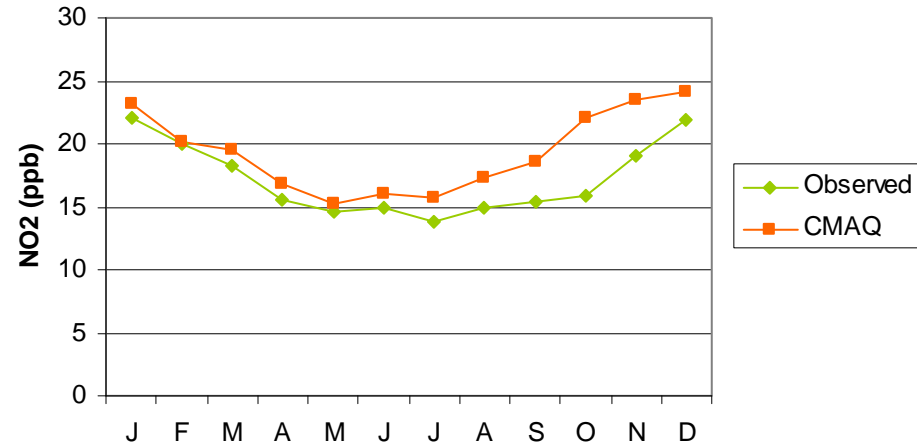
6-9 am NOx/TNMOC ratio, June-August

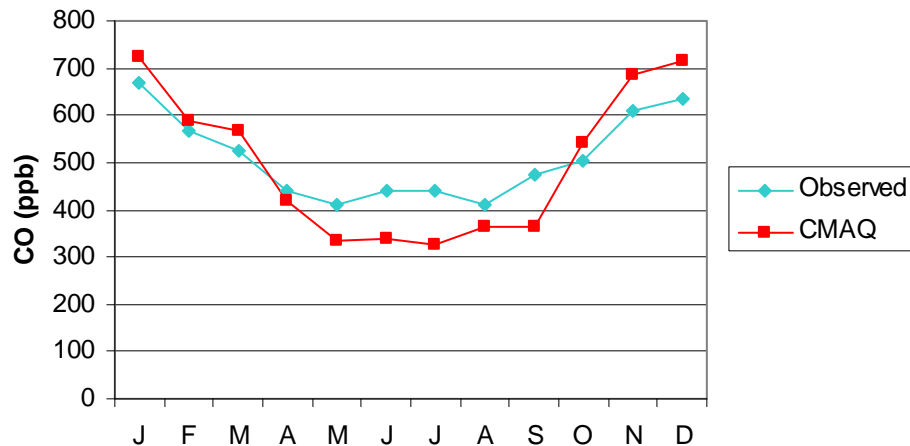6-9 am NOx, TNMOC, and NOx/TNMOC ratios

Monthly variation of trace gases
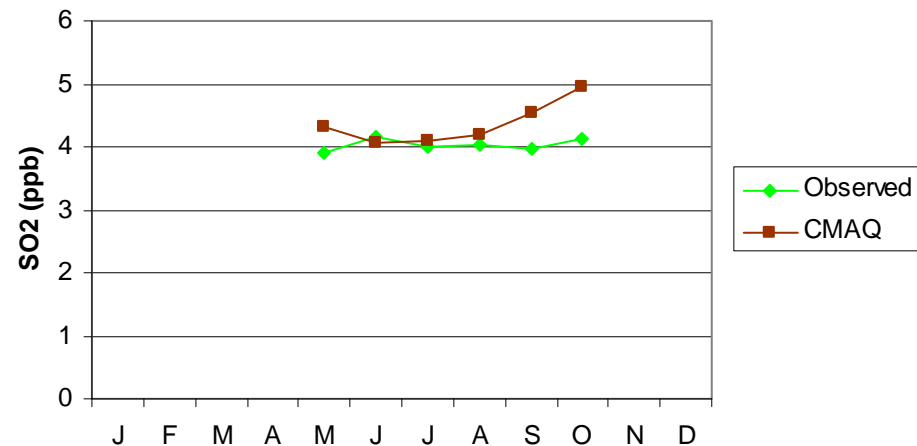
Selected statistical measures for daily maximum 8-hour O$_3$ in the Albany-Schenectady-Troy, NY nonattainment area
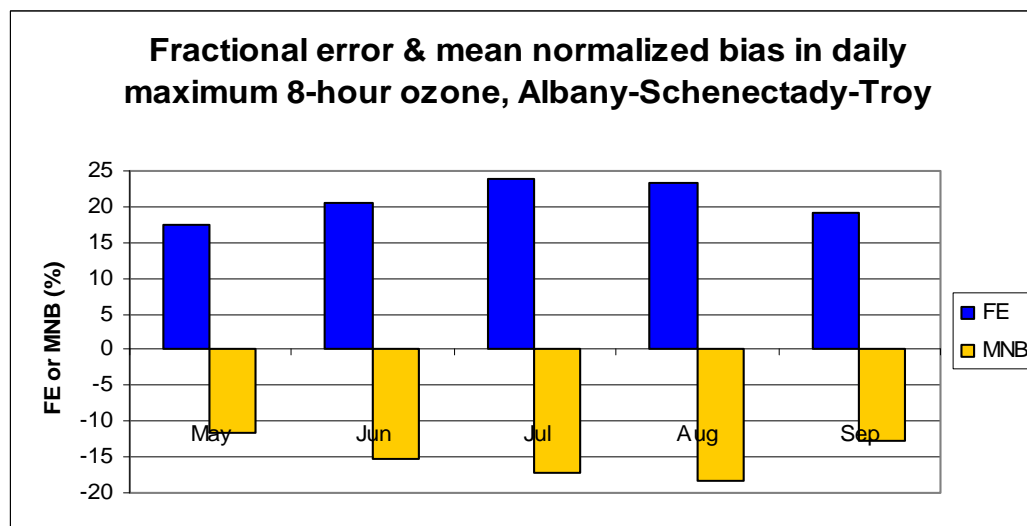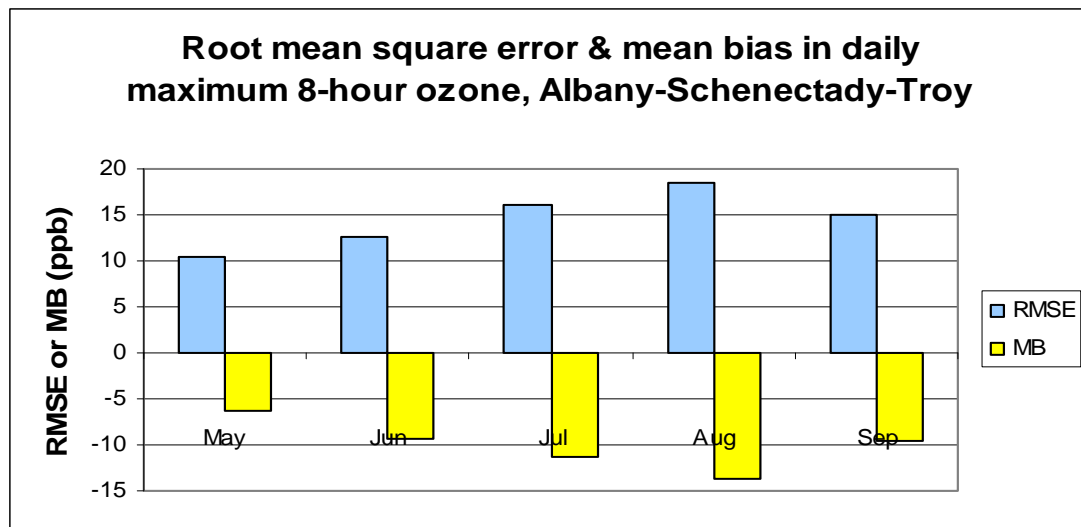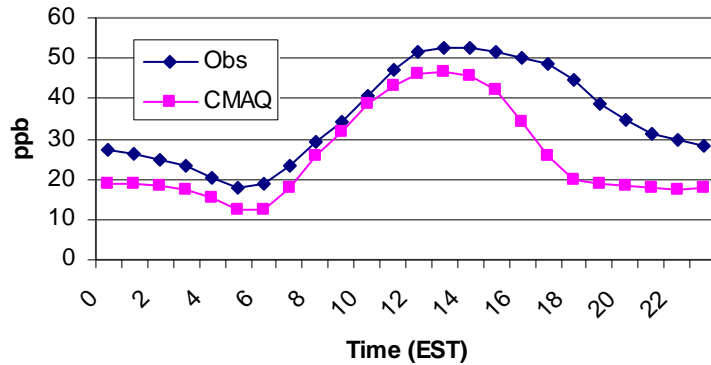
Root mean square error & mean bias in daily maximum 8-hour ozone, Albany-Schenectady-Troy

Fractional error & mean normalized bias in daily maximum 8-hour ozone, Albany-Schenectady-Troy
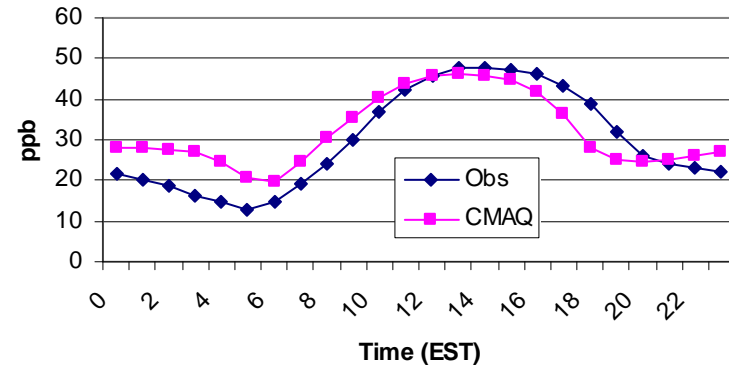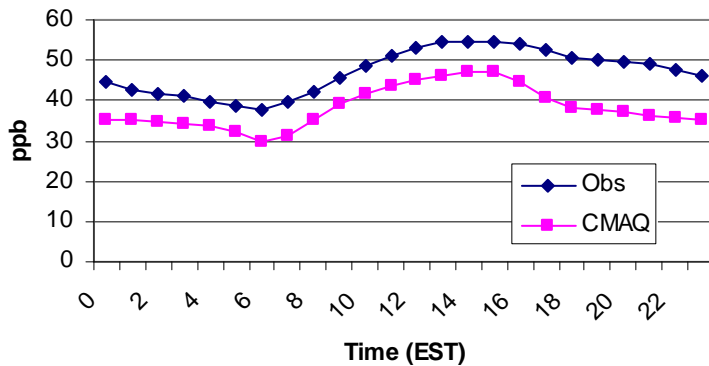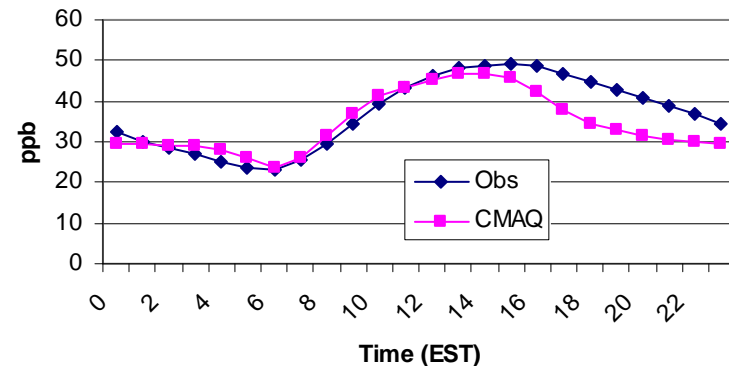
Diurnal variation at four ozone monitors in the
Albany-Schenectady-Troy, NY nonattainment area

| MASSACHUSETTS PERFORMANCE STATISTICS FOR 2002 CAA CMAQ RUN (OTB/OTW plus CAIR)						
Location	AIRS ID	Mean Normalized Gross Error %			Mean Normalized Bias %	
		1 hr daily max	8 hr daily max		1 hr daily max	8 hr daily max
Truro	250010002	15.2	15.0		8.2	9.7
Adams	250034002	14.7	14.6		-6.2	-7.3
Fairhaven	250051002	14.2	15.6		5.3	6.1
Lawrence	250090005	17.7	17.0		2.4	0.8
Lynn	250092006	16.6	17.6		-7.5	-8.5
Newbury	250094004	16.2	16.4		8.8	8.6
Agawam	250130003	17.7	16.2		-7.6	-8.8
Chicopee	250130008	17.2	16.6		-11.7	-12.4
Amherst	250150103	15.5	14.3		-3.3	-2.1
Ware	250154002	14.4	14.4		-6.7	-6.6
Stow	250171102	16.8	14.9		-2.1	-5.4
Milton	250213003	18.8	23.0		-15.9	-20.6
Boston (Long Island)	250250041	19.1	22.4		-10.5	-15.4
Boston	250250042	21.6	26.6		-18.9	-24.3
Ware	250270015	18.5	17.5		-7.2	-10.1
		16.9	17.5		-4.9	-6.4

Maryland Analyses

- Extremely good simulation of 1-hr (8-hr) maximum O_3 R>0.9

- CMAQ-calculated O_3 concentrations have high bias at night leading to a 10% high-bias in 24-hr average O_3.   Biases in 1-hr and 8-hr maximum O_3 are small.

- CMAQ-calculated 1-hr maximum O_3 concentrations over MD are 10-15% too low during major pollution events.

- Diurnal variation in O_3 well simulated. No obvious (eyeball norm) temporal shift in timing of maxima/minima.

- Spatial pattern of O_3 pollution events is well captured by CMAQ.
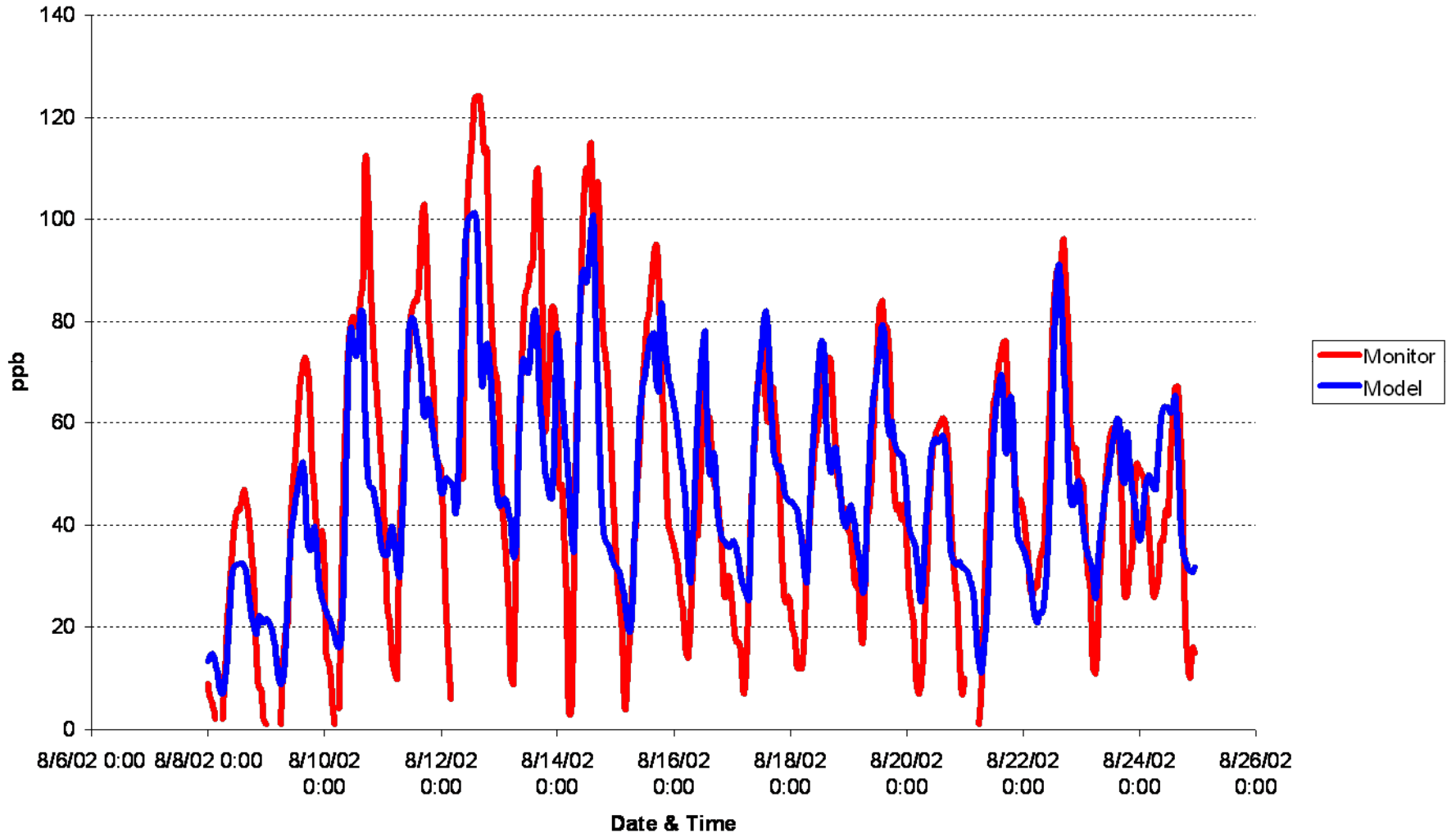
Maryland Analyses (in progress)

- Comparison of CMAQ-calculated O_3 concentrations with UMD aircraft data

- Comparison of CMAQ-calculated $PM_{2.5}$ concentrations with measurements during non-summer seasons

- Comparison of CMAQ-calculated NO and SO_2 with measurements

- Comparison of $PM_{2.5}$ components (sulfate, nitrate, ammonium, elemental carbon, soil/crustal organic) with measurements

PA Analysis: 8-hr Max R^2 Values

Legend

8-Hour Max R^2

○ 0.00

○ 0.01 - 0.55

○ 0.56 - 0.65

○ 0.66 - 0.70

● 0.71 - 0.78

80   40   0   80 Miles
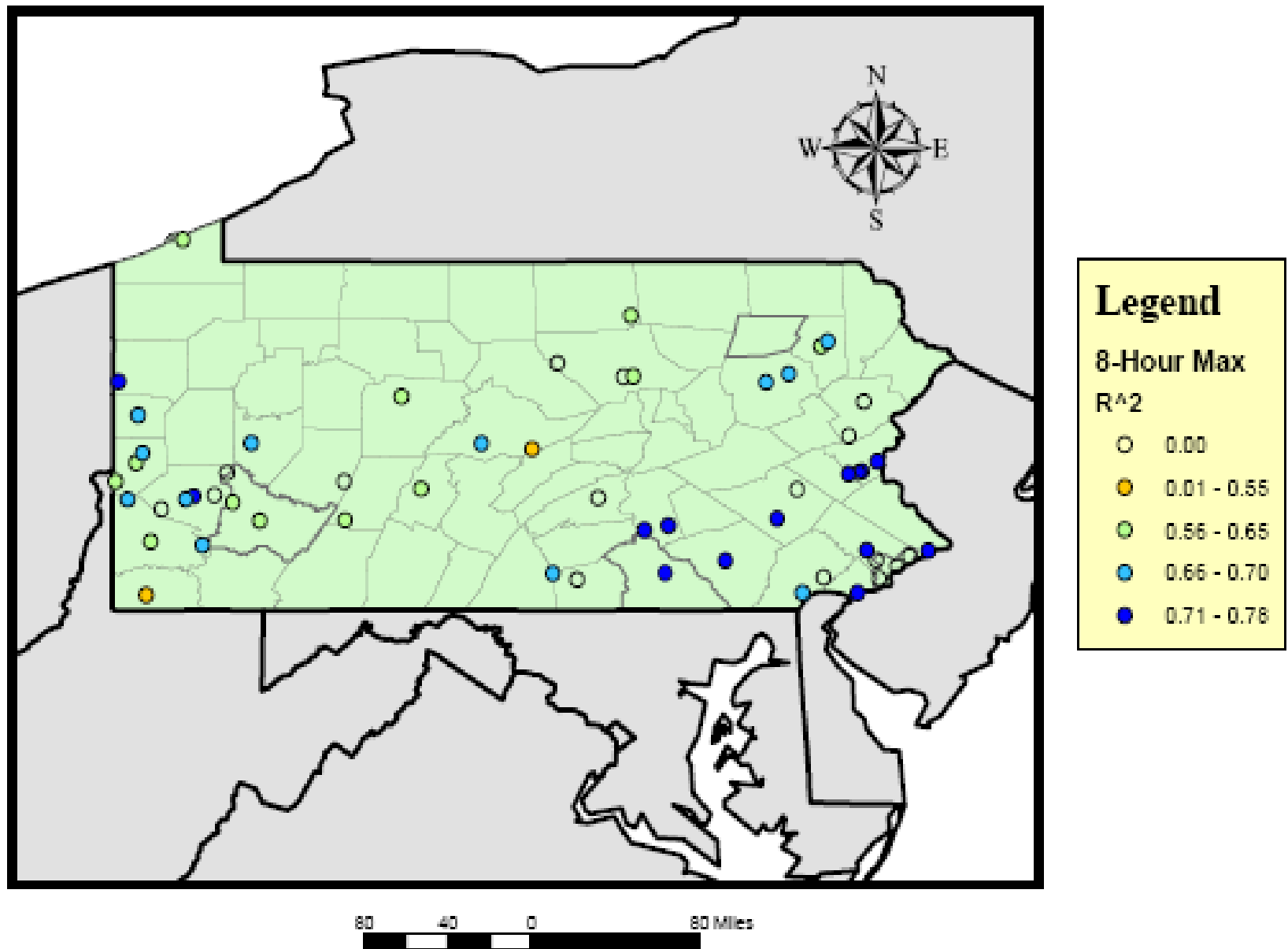
Lancaster Monitor

2002 Hourly Ozone Comparison
Lancaster 8/6/02 to 8/26/02

Lancaster Analysis

Good:

   R^2: Model doing a good job over all.

   Correlation: Model directionally good.

   Solar Rad Correlation: Model doing well during daylight hours (when max occurs).

Bad:

   Coefficient of Divergence: Significant difference in absolute model concentrations overall. These are generally confined to the overnight hours (may not be not as important).

Well Simulated Plume from VA to CT

Daily Maximum 8-hr Ozone Concentrations, Predicted
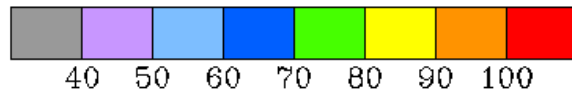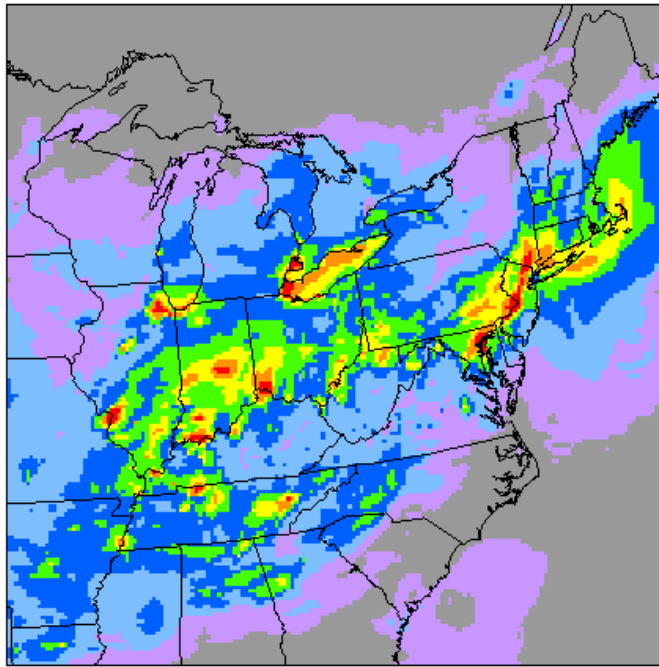Tuesday, 06/11/2002, Maximum =129.4 ppb
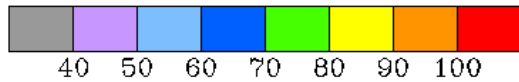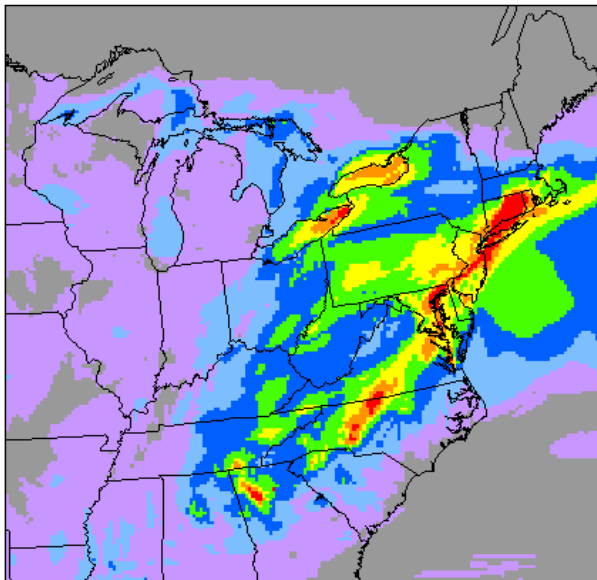
Daily Maximum 8-hr Ozone Concentrations, Observed
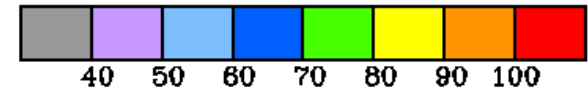Tuesday, 06/11/2002, Maximum =123 ppb
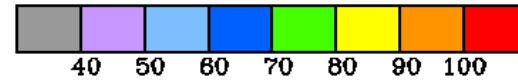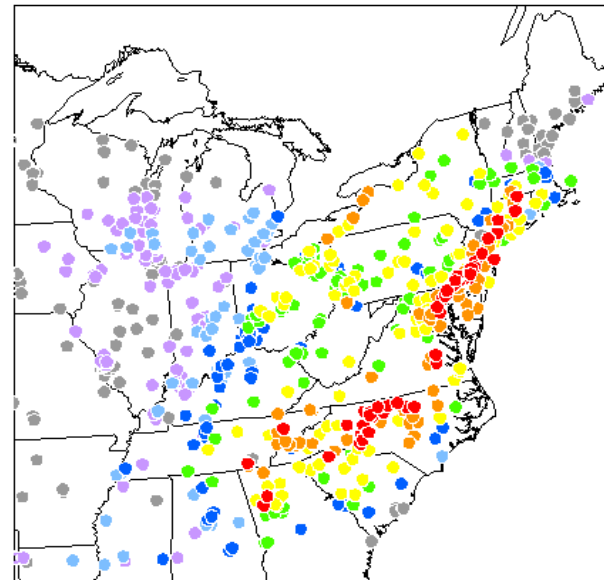
Narrow band of high ozone from Maryland to southwest New England Well Simulated

Daily Maximum 8-hr Ozone Concentrations, Predicted
Sunday, 08/04/2002, Maximum =121.2 ppb

Daily Maximum 8-hr Ozone Concentrations, Observed
Sunday, 08/04/2002, Maximum =117 ppb
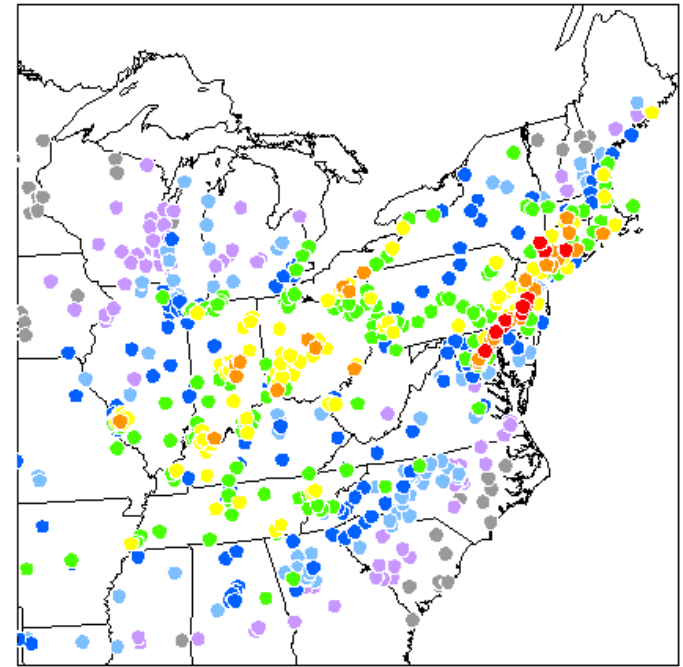
Expansive Area of Elevated Ozone; Well Simulated Clean Marine Influence along all but Northern New England Coast; Seabreeze Transport of Ozone along N. New England Coast Well Simulated

Daily Maximum 8-hr Ozone Concentrations, Predicted
Tuesday, 09/10/2002, Maximum =114.0 ppb
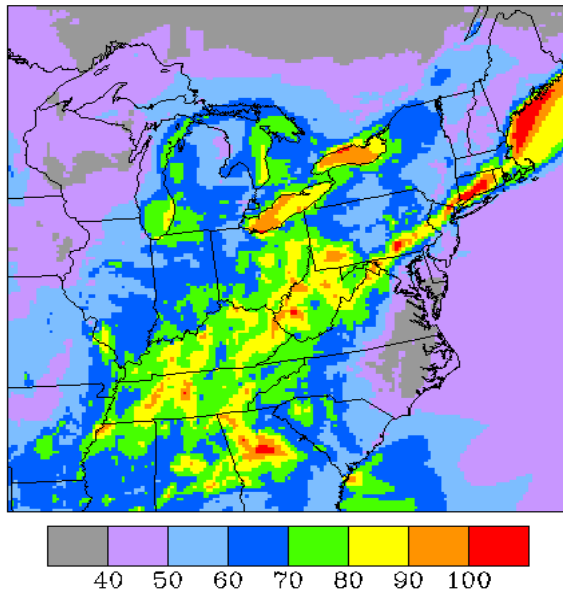
Daily Maximum 8-hr Ozone Concentrations, Observed
Tuesday, 09/10/2002, Maximum =119 ppb
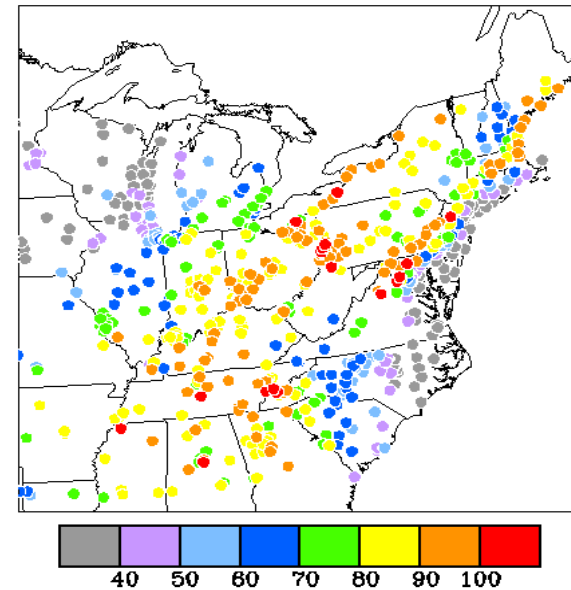
Summary

- Spatial patterns of observed and simulated daily maximum 8-hour ozone exhibit good agreement

- Model has tendency to underpredict the observed ozone maxima

- Fair agreement is noted between measured and predicted daily maximum concentrations for other pollutants

What's Next?

- States are working with MARAMA to compile the base case emission inventory for 2009

- NYSDEC is setting up 2009 CAA Modeling Run (OTB/OTW plus CAIR)

- States are working to identify potential state and regional level control strategies that may be necessary for demonstrating attainment of the 8-hour ozone NAAQS

2009 CAA (OTB/OTW plus CAIR) Run

MANEVU 2009 Emission Files (OTB/OTW plus CAIR) - late November

Other RPOs 2009 Emission Files (OTB/OTW plus CAIR) - late November

Canada 2009 Emission Files (or surrogate) – late November

2009 (OTB/OTW plus CAIR) CMAQ Simulation - late December

2009 (OTB/OTW plus CAIR) Projected Design Values – mid January

OTB means on the books
OTW means on the way and effective by 2009
CAIR means EPA's Clean Air interstate Rule

Participants in OTC Modeling Effort

Maryland Department of the Environment (MDE)

Mike Woodman and Tad Aburn

University of Maryland at College Park (UMD)

Jeff Stehr, Sheryl Ehrman, Dale Allen, Dalin Zhang, Shunli Zhang

Virginia Department of Environmental Quality (VADEQ)

Shiang-Yuh Wu, Mike Kiss, Jin-Sheng Lin, Tom Ballou

New Jersey Department of Environmental Protection (NJDEP)

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Northeast States Consortium of Air Use Management (NESCAUM)

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