Regional Air Quality Forecasts during NEAQS-2K2: Comparisons with Observations

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Comparisons of Two Real-time Air Quality Models, MMM5-CHEM and MAQSIP-RT

Focus on O_3 photochemistry within the Northeast U.S.

- **Characterize O_3 predictions - two statistical measures**
- **Emissions from observations and model results**
- **Photochemical mechanisms - O_3 formation**

Air Quality Forecast Web Sites

NOAA/FSL: http://www-frd.fsl.noaa.gov/aq/wrf
BARON AMS: http://www.baronams.com/products/maqsip

Summary of MAQSIP-RT and MM5-CHEM Eulerian Forecast Models
for the NEAQS-2002 study

	MCNC MAQSIP-RT	FSL MM5-CHEM
Model Resolution	45, 15, 5 km	27, 9, 3 km
Formulation	Offline (1/2 hr)	Online
Emissions	SMOKE	EPA-NET96 (county level)
Chemistry	CB-IV	RADM-2
BL physics	MRF physics	Mellor-Yamada2.5
Met. Initialization	ETA 22-km	RUC 20-km (12 hr spin-up)
Structure	30m lowest level	15m lowest level
Convection	All 3 resolutions Kain-Frisch	Only 27 km resolution Grell et al., 2001

- **Although both models are based on MM5, there is no similarity**
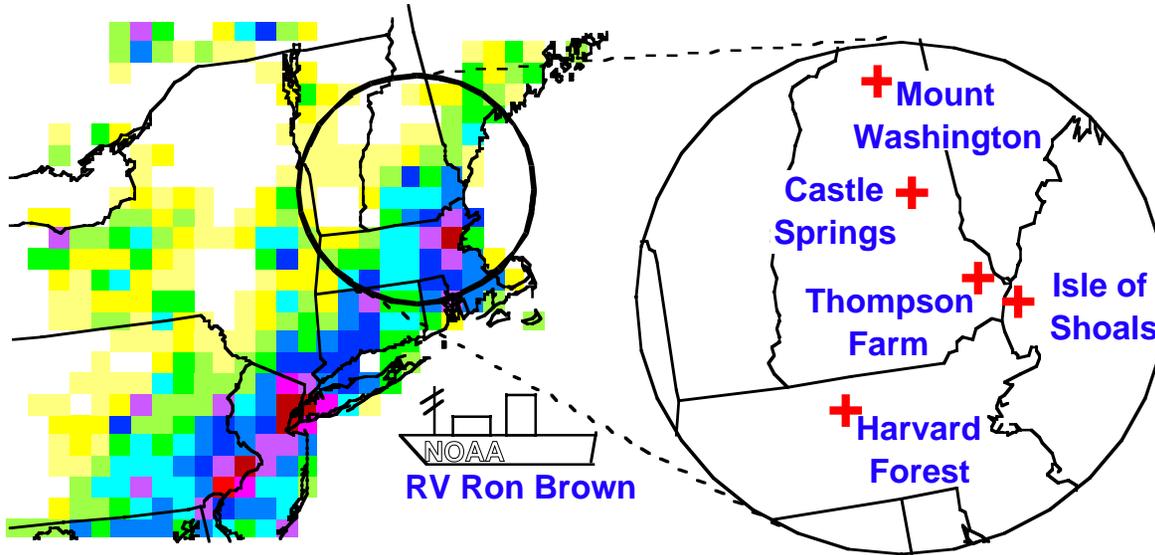
EPA NET-96 (version 3.11)

NOx emissions, all sources, 27 km resolution

5.0 7.5 11.2 16.9 38. 25.3 57. 85.4 128.1 192.2 288.3 432.5 1149

10^{14} molec-m^{-2}-s^{-1}

• Focus only on O_3, NOy and CO

• Emissions for course resolution models inadequate near coastlines
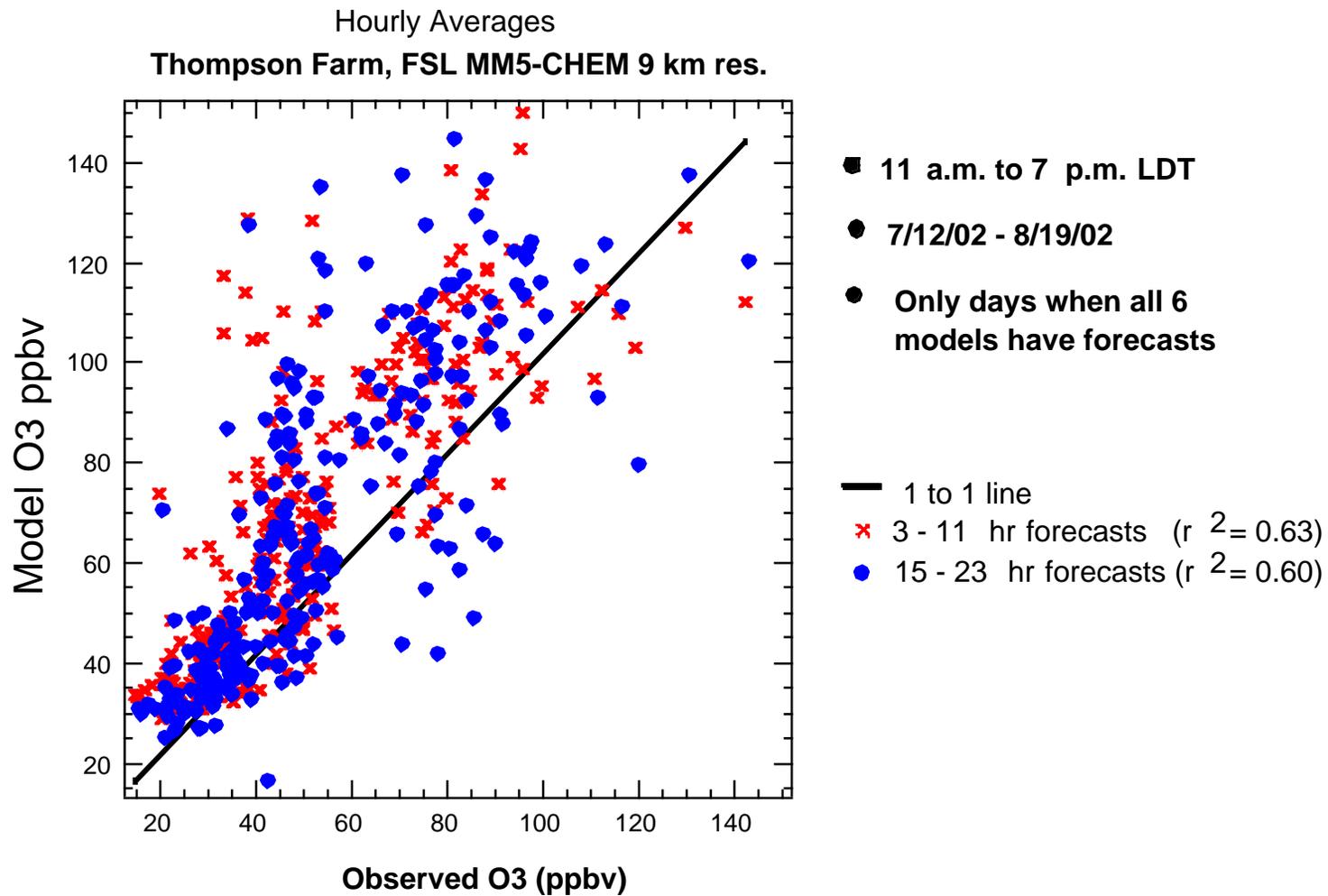
RV Ron Brown - O_3, NOy, SO_2, NOx

Isle of Shoals - O_3, CO

Thompson Farm - O_3, CO, NOy, SO_2, NOx

Castle Springs - O_3, CO, NOy, SO_2, NOx

Mount Washington - O_3, CO, NO, SO_2

Harvard Forest - O_3, NOy, CO, PAN, NOx

Hourly Averages
Thompson Farm, FSL MM5-CHEM 9 km res.

11 a.m. to 7 p.m. LDT

7/12/02 - 8/19/02

Only days when all 6 models have forecasts

— 1 to 1 line
× 3 - 11 hr forecasts ($r^2 = 0.63$)
● 15 - 23 hr forecasts ($r^2 = 0.60$)

● **Pearson r^2 value used as a measure of forecast skill**

● **No difference in r^2 for different forecast start times**

Hourly Averages
Thompson Farm, FSL MM5-CHEM 9 km res.
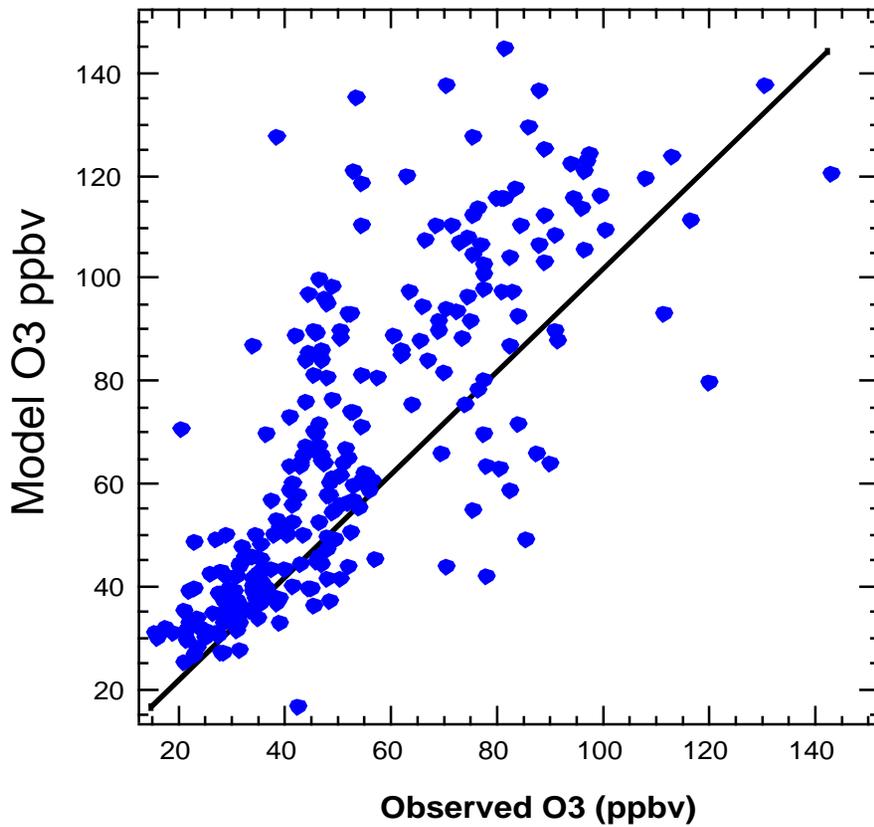
8 Hour Averages (11 am - 7 pm LDT)
Thompson Farm, FSL MM5-CHEM 9 km res.

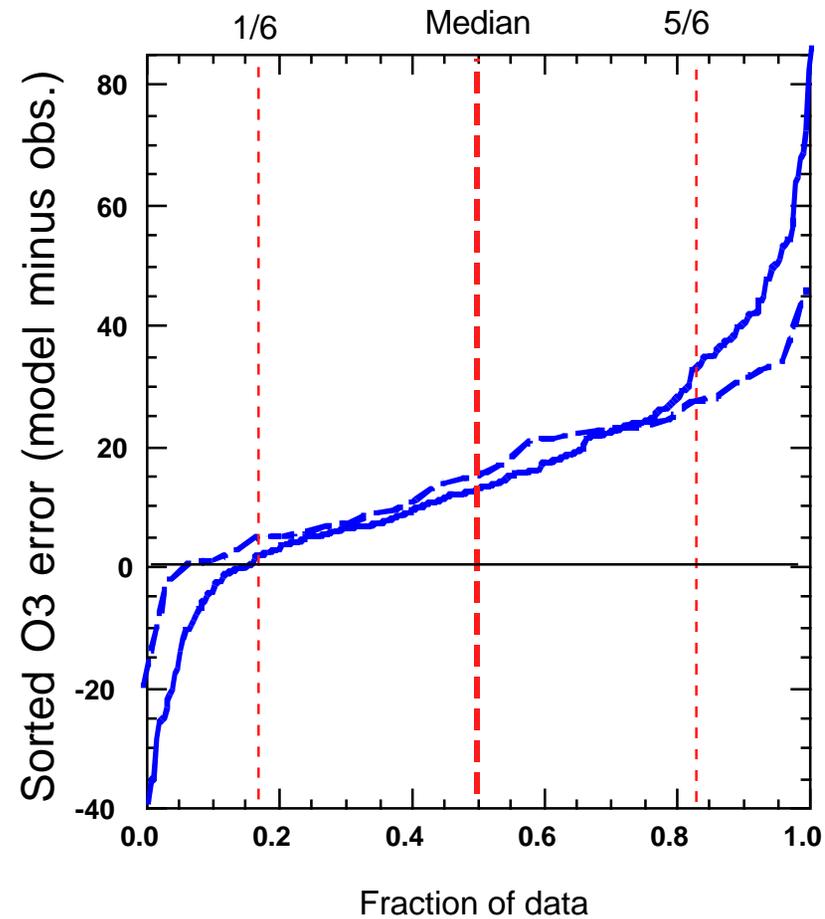— 1 to 1 line

● 15 - 23 hr forecasts ($r^2 = 0.60$)
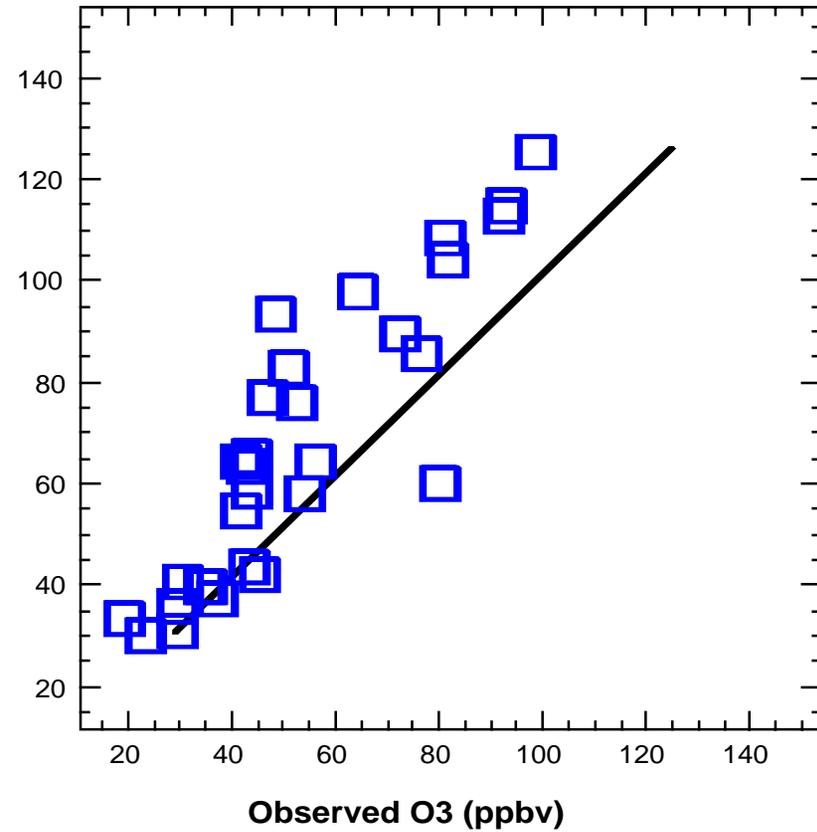
☐ 15 - 23 hr forecasts ($r^2 = 0.79$)

● **Analysis restricted to first 23 hours of 00Z forecasts**

● r^2 **of 8 hour averages used as a measure of day-day, large-scale forecast ability**

● r^2 of 8 hour averages always > r^2 of 8 hour averages
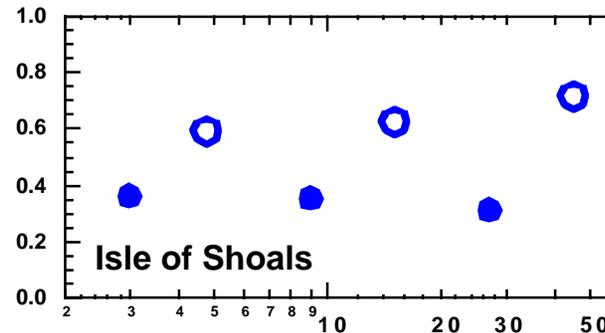
Hourly Averages
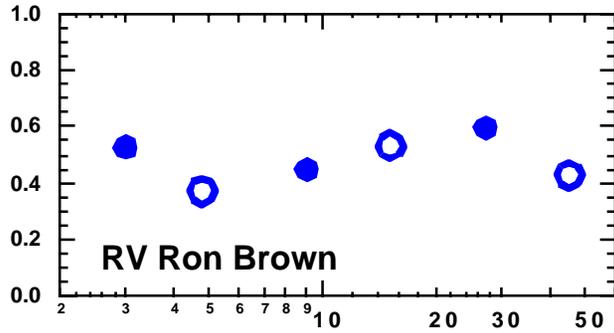**Thompson Farm, FSL MM5-CHEM 9 km res.**

Model O3 ppbv — Observed O3 (ppbv)

Sorted O3 error (model minus obs.) — Fraction of data

1/6   Median   5/6
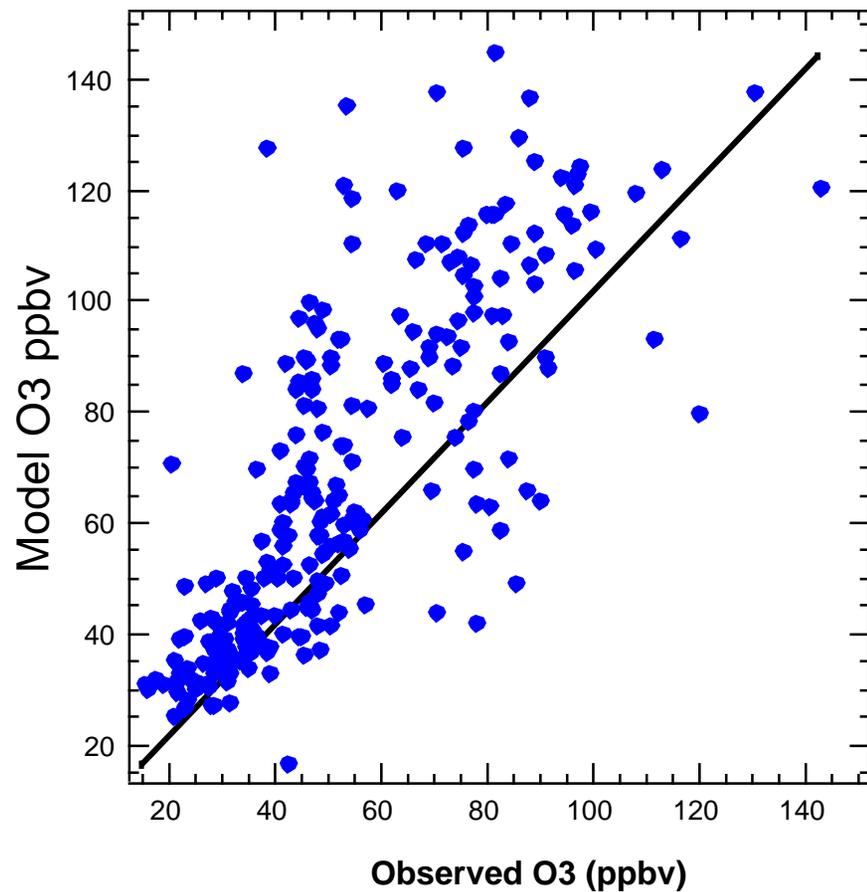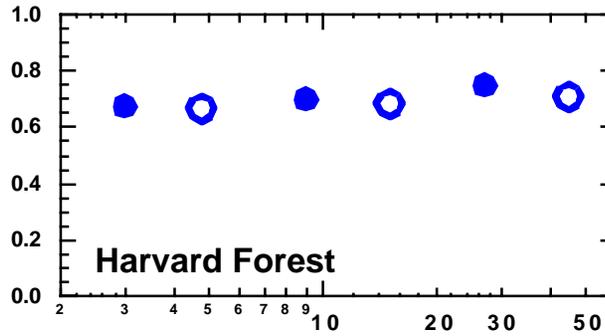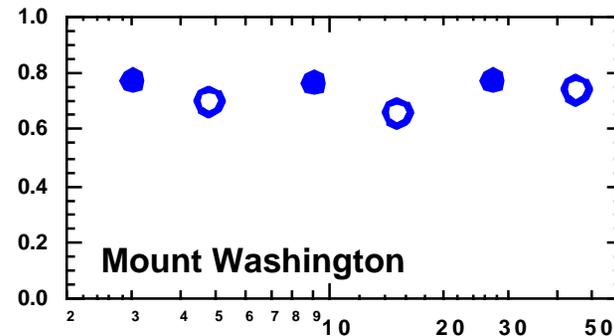
—— 1 to 1 line
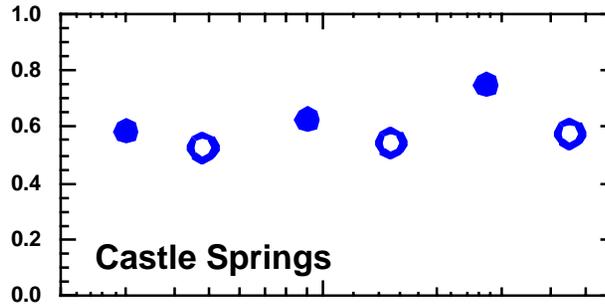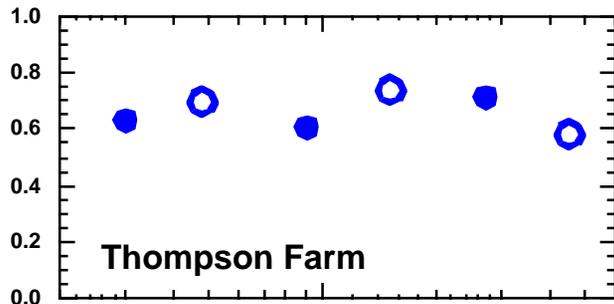
● 15 - 23 hr forecasts ($r^2 = 0.60$)

—— 1 hr averages
---- 8 hr averages

● **Median model bias used as the second statistical measure**

● **Median model biases the same for 8 hr averages and 1 hour averages**

O$_3$ r^2 correlation coefficients

Legend:
- ○ MAQSIP-RT, hourly avgs.
- ● MM5-CHEM, hourly avgs.

Panels (x-axis: Model horizontal resolution (km)):
- RV Ron Brown
- Isle of Shoals
- Thompson Farm
- Castle Springs
- Mount Washington
- Harvard Forest
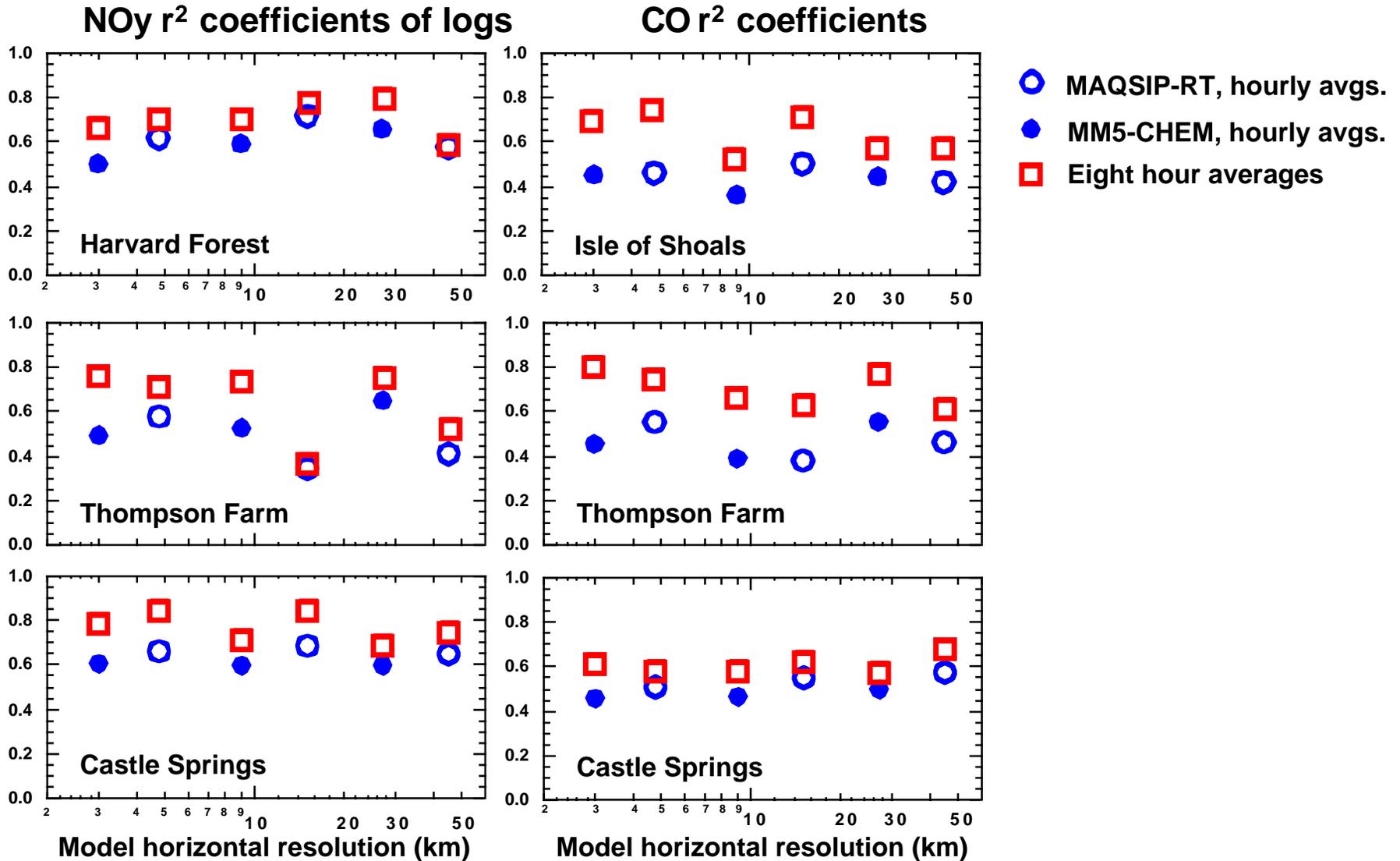
- **No apparent improvement of forecast skill as model resolution increases**
- **Except at Isle of Shoals, one model not any better than the other**

O$_3$ r^2 correlation coefficients

- MAQSIP-RT, hourly avgs.
- MM5-CHEM, hourly avgs.
- Eight hour averages

RV Ron Brown

Isle of Shoals

Thompson Farm

Castle Springs

Mount Washington

Harvard Forest

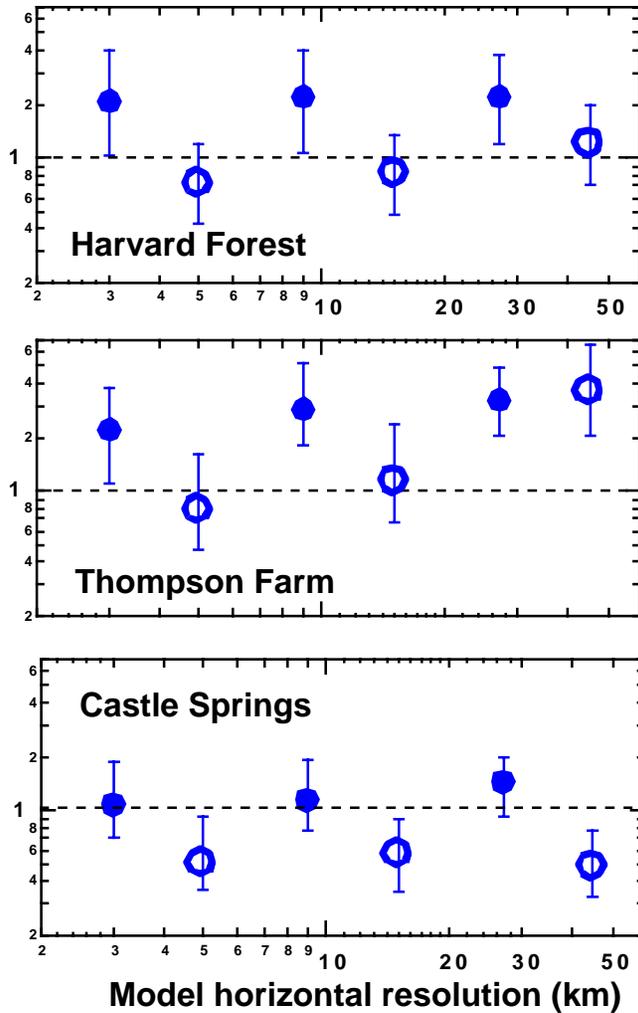Model horizontal resolution (km)
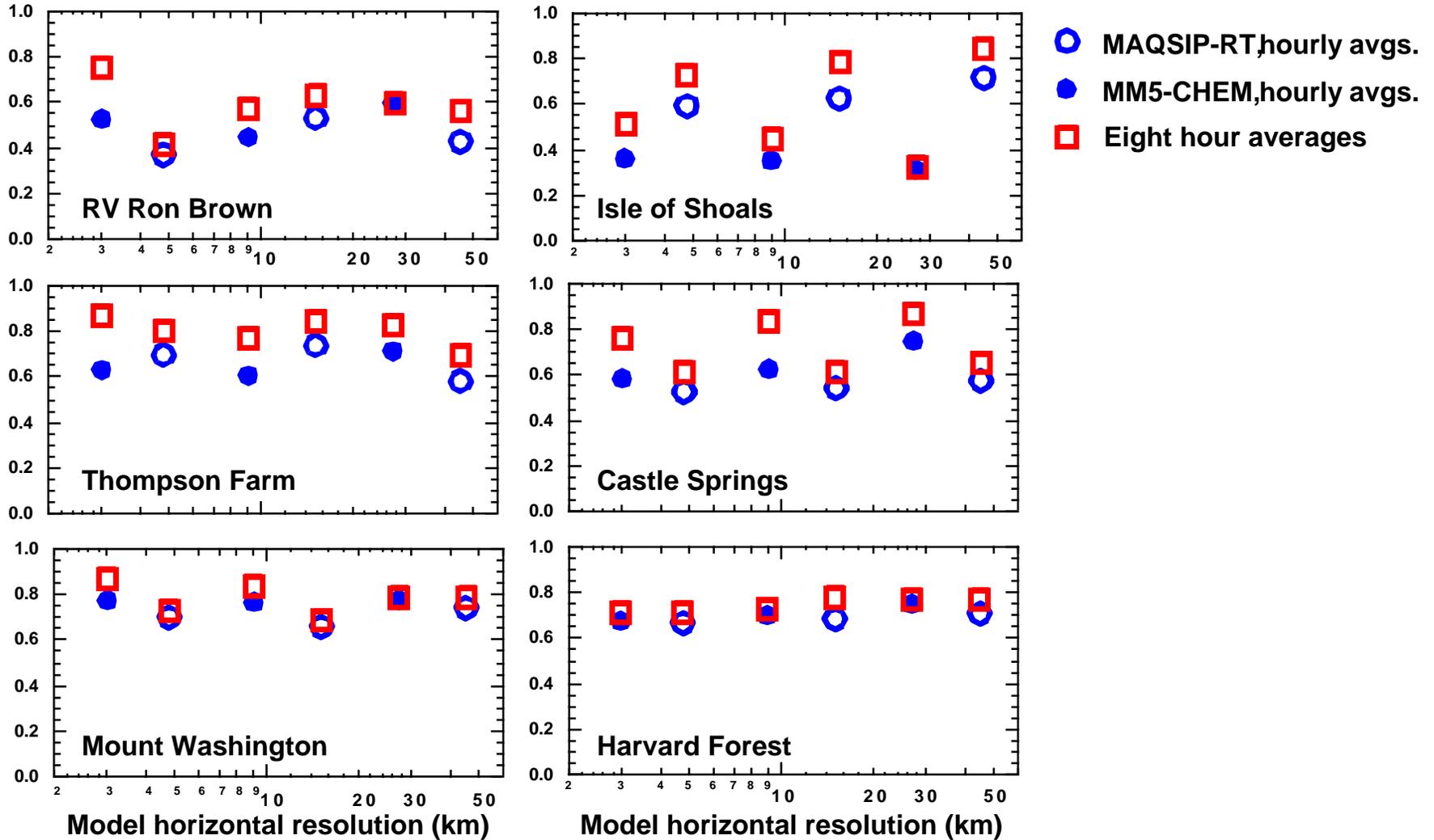
- **Correlations of hourly averages driven by day-to-day, larger scale correations**
- **MM5-CHEM does relatively worse at handling diurnal variability at TF and CS**
- **No significant trends in O$_3$ bias with model resolution, MM5-CHEM higher**

NOy r² coefficients of logs

CO r² coefficients

Legend:
- MAQSIP-RT, hourly avgs. (open blue circle)
- MM5-CHEM, hourly avgs. (filled blue circle)
- Eight hour averages (open red square)

Left column panels: Harvard Forest, Thompson Farm, Castle Springs
Right column panels: Isle of Shoals, Thompson Farm, Castle Springs
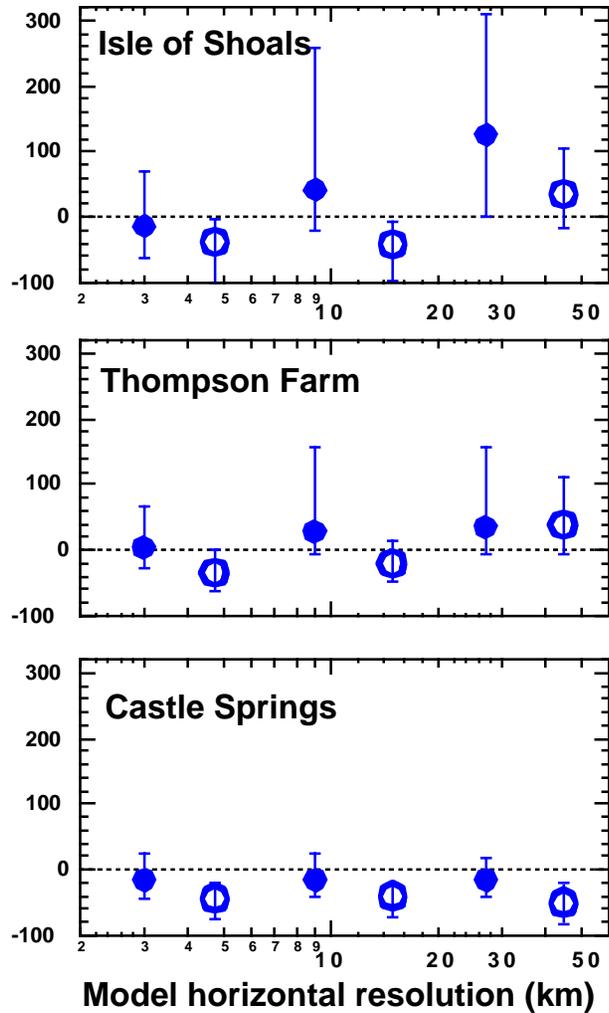
X-axis: Model horizontal resolution (km)

- Both models do diurnal variability worse for coastal sites, for both NOy and CO
- No improvement in forecast skill with increasing model resolution
- For 8 hr averages, improvement of skill with higher resolution

NOy median model/obs.

CO median model error (ppbv)

Harvard Forest

Thompson Farm

Castle Springs

Isle of Shoals

Thompson Farm

Castle Springs

Model horizontal resolution (km)

○ MAQSIP-RT, hourly avgs.
● MM5-CHEM, hourly avgs.

• Some improvements in model biases as resolution increases
• MM5-CHEM biased high by a factor of 2
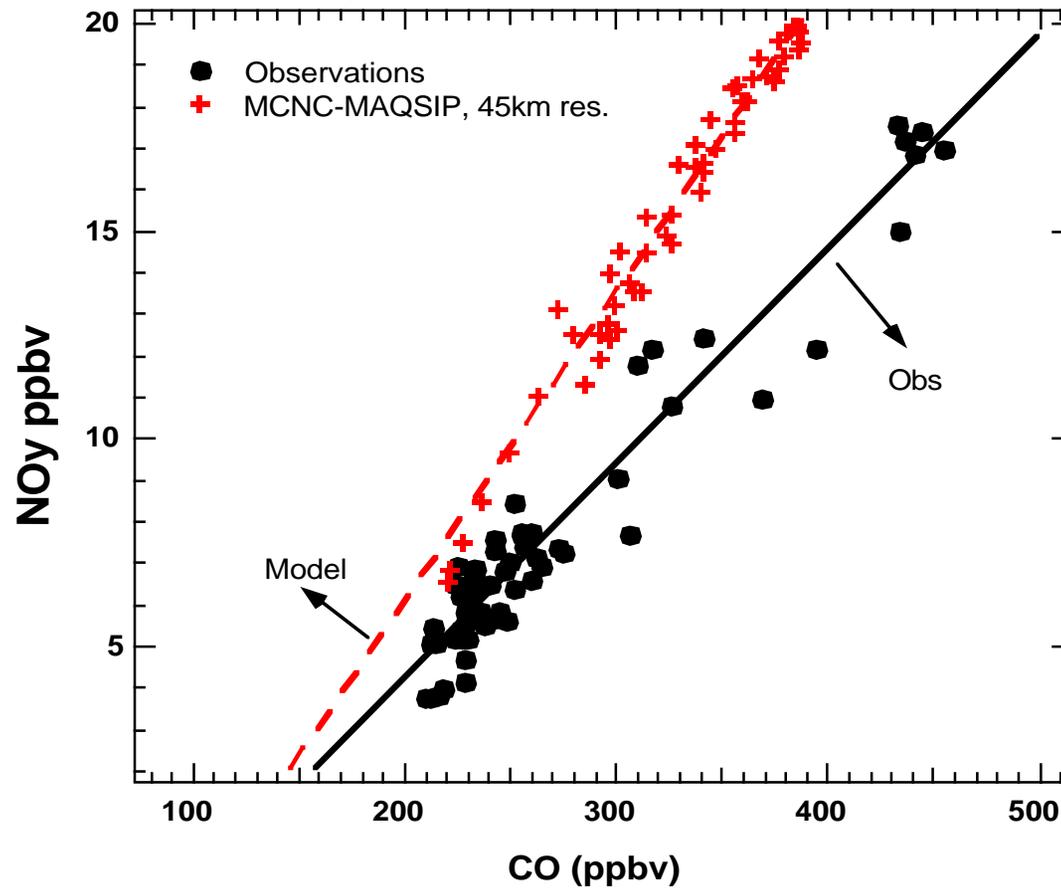• MM5_CHEM biased high relative to MAQSIP for all cases of NOy and CO

Harvard Forest, averages at 20Z
7/13/02 - 8/19/02
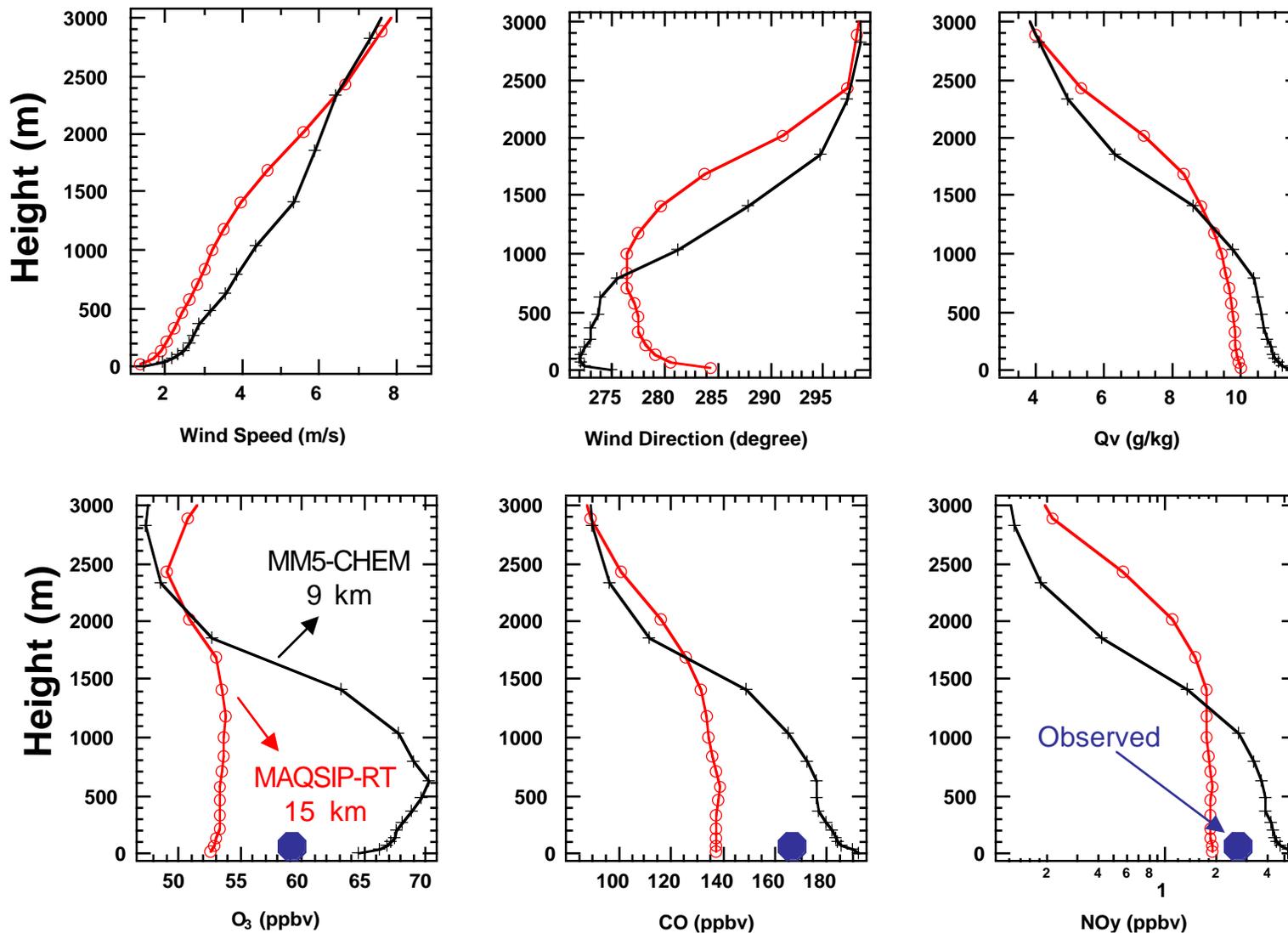
- MAQSIP has much deeper and faster mixing of O_3, NO_y, CO and H_2O
- Bottom 200 meters suggest slower MM5-CHEM transport from surface

Emissions Ratios from
Species-Species Correlations
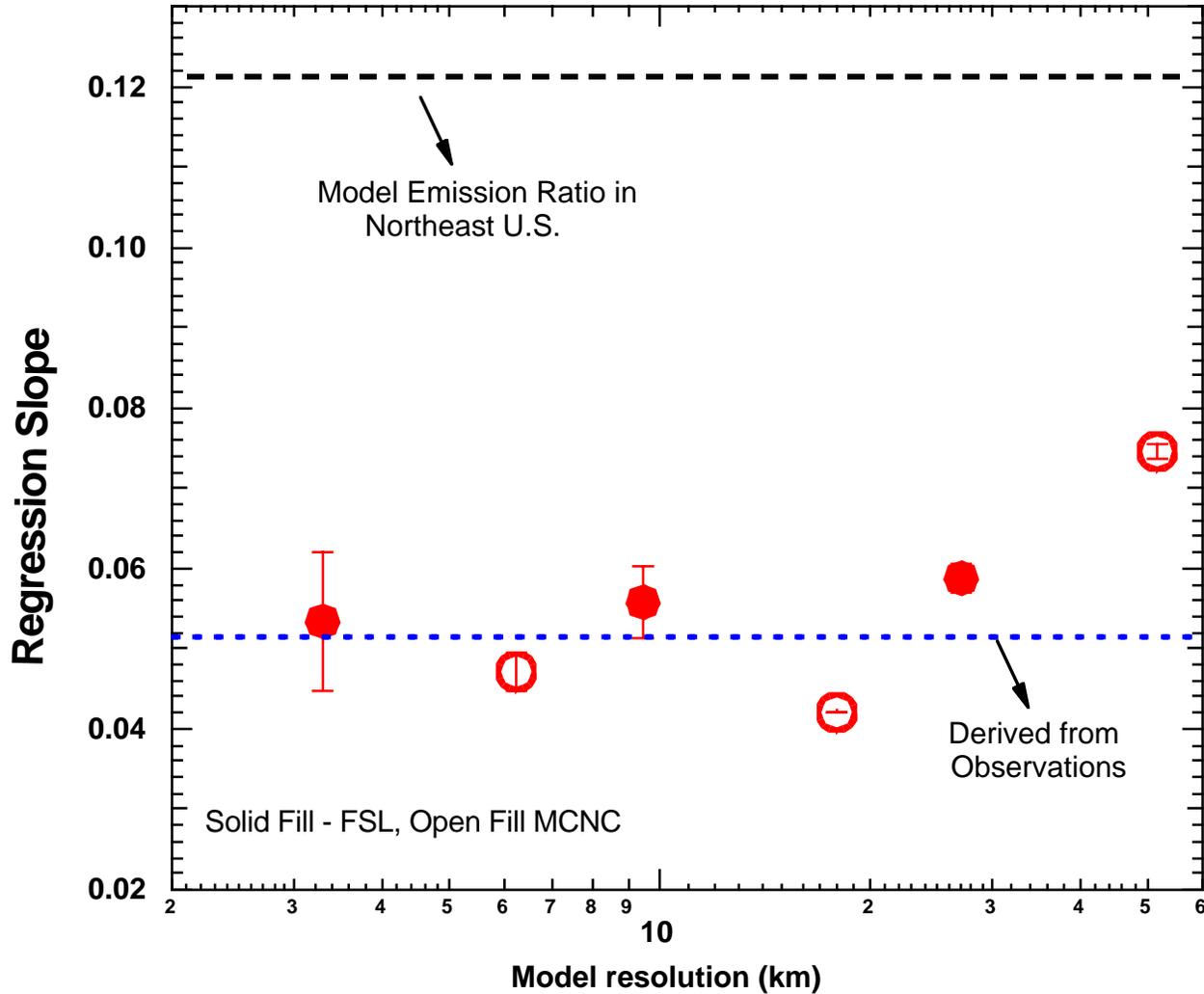
Thompson Farm, NH, 8/13/02 - 8/15/02

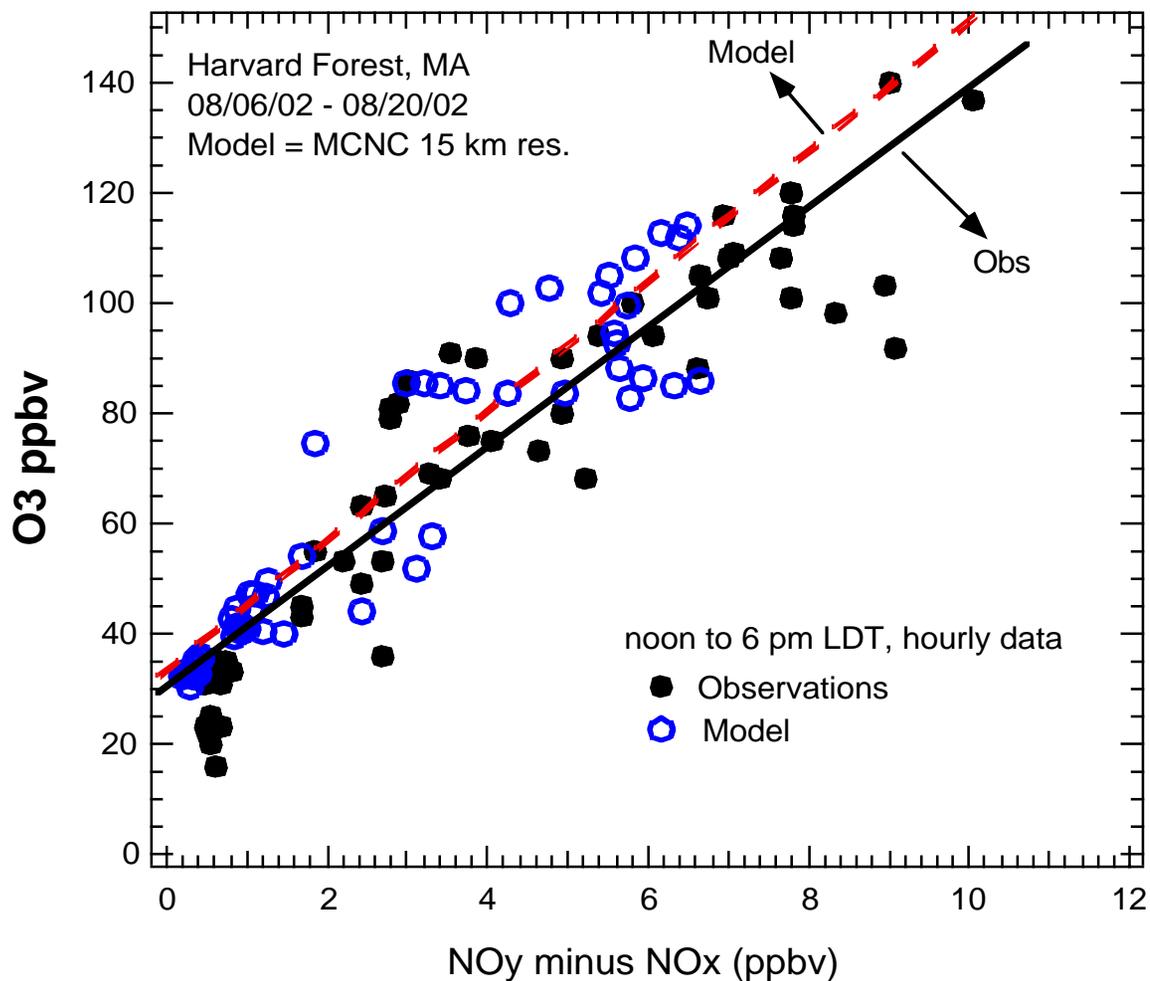
Observed Slope = .051 +/- .002
Model Slope = .074 +/- .001

•High Correlations between NOy and CO for specific episodes

Thompson Farm, 8/13/02 - 8/15/02
NOy/CO ratios from regression slopes

- NOy to CO ratios predicted extremely well (for this case)
- Model ratios a factor of 2 below emission ratios
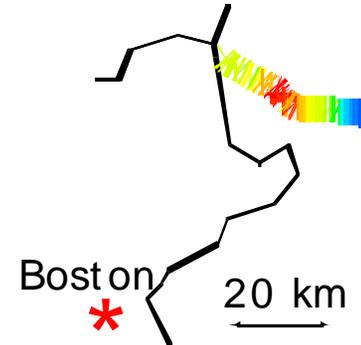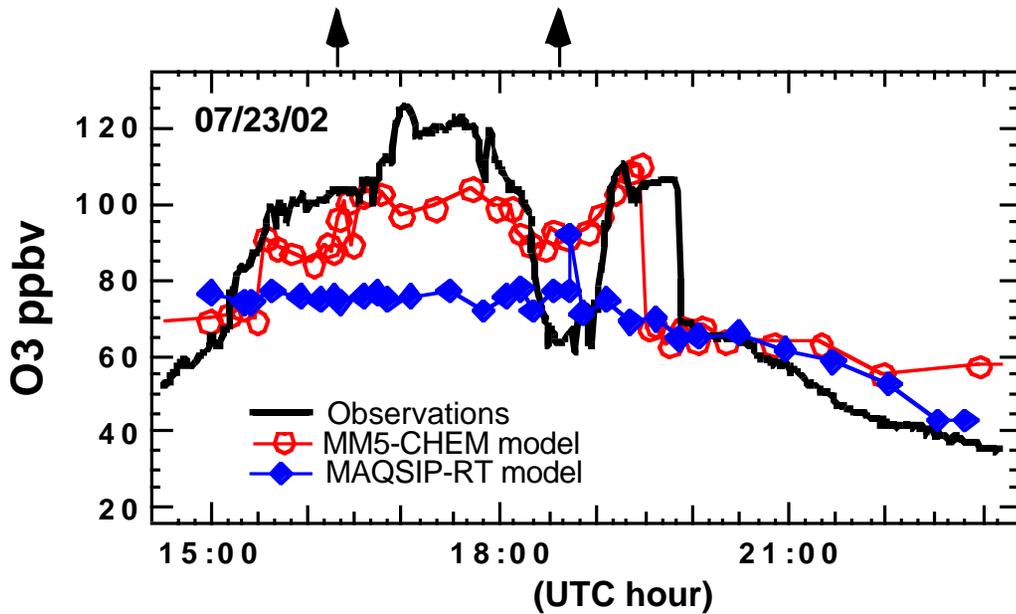- Deposition of NOy a controlling factor in ratio determination

Ozone Production Efficiency
From observations and model results

Harvard Forest, MA
08/06/02 - 08/20/02
Model = MCNC 15 km res.

Model

Obs

noon to 6 pm LDT, hourly data
● Observations
○ Model

NOy minus NOx (ppbv)

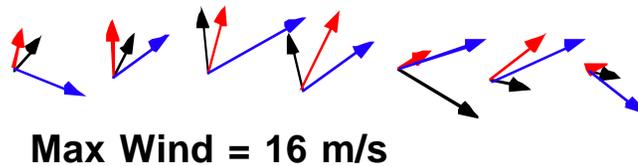Observed Slope = 10.8 +/- .3
Model Slope = 11.7 +/- .4

•Ozone versus NOy-NOx as a measure of ozone production efficiency
•Good correlations for the Harvard Forest site, 14 days in August

07/23/02

O3 ppbv

120
100
80
60
40
20

15:00   18:00   21:00

(UTC hour)

— Observations
—○— MM5-CHEM model
—◆— MAQSIP-RT model

Max Wind = 16 m/s

Boston
20 km

16:20 to 18:40   UTC

Red = 120 ppbv
Blue = 60 ppbv

• MAQSIP-RT missed the plume transport and frontal boundary

•MM5-CHEM captured frontal boundary, ozone plume and ozone production efficieny

O3 ppbv

120
100
80
60

2   4   6   8   10

NOy minus NOx (ppbv)
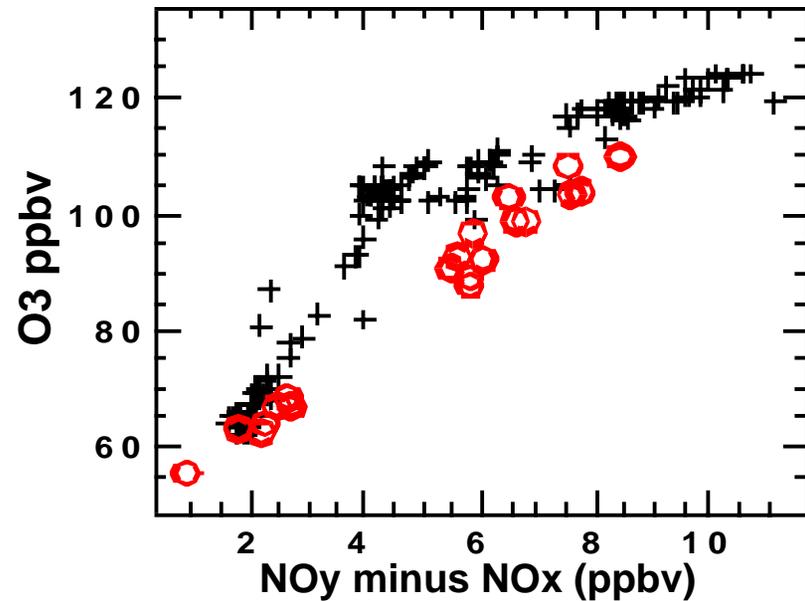
Conclusions

*   **MM5-CHEM versus MAQSIP-RT comparisons**

    No big advantage to finer horizontal resolution

    Emission ratios (CO/NOy) reproduced well

    O_3 production efficiency reproduced well

    Large influence of NOy deposition in model correlations

    Biases can be attributed to PBL transport differences

Comparisons of models that will be operational in 2004

*   WRF-CHEM-Aerosol (FSL/NOAA)

    Steve Peckham et al.

    Lisa Darby et al.

    NEAQS 2K2 poster session

*   ETA-CMAQ (NWS/NCEP/ARL)

    See Stu McKeen