



# **NCEP Air Quality Forecast System Upgrades for the Summer 2005**

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Bert Katz, Geoff Manikin and Sarah Lu**

***\*NOAA/NCEP***

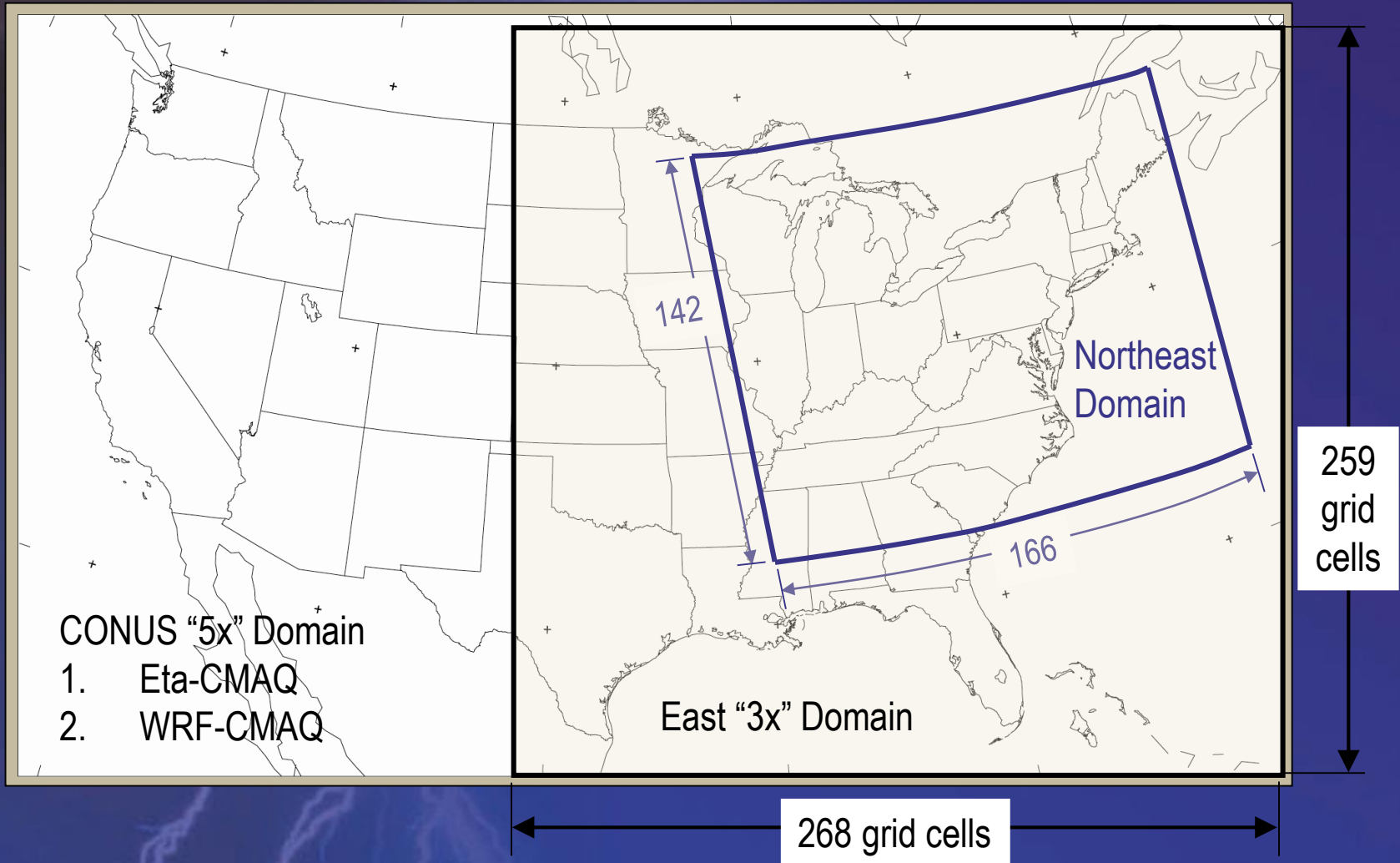
***Environmental Modeling Center***

***Rohit Mathur, Daiwen Kang, Shoicai Yu and Hsinn-Mu Lin***  
***NOAA/ARL and EPA/ASMD***

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# Forecast Domains (2005)



# Upgraded Air Quality Forecasting Configuration for Operational NE US Domain

- **NE Domain**: 48 hour forecasts of ozone ( $O_3$ ) : 06 and 12 UTC runs

- 12 km 166x142x22 top at 100 mb

- Optimized PREMAQ/CMAQ codes

- New NAM landuse definitions for deposition effects

- ✓ Updated emissions inventories:

- ✓ Project 2002 point and area source inventories for 2005

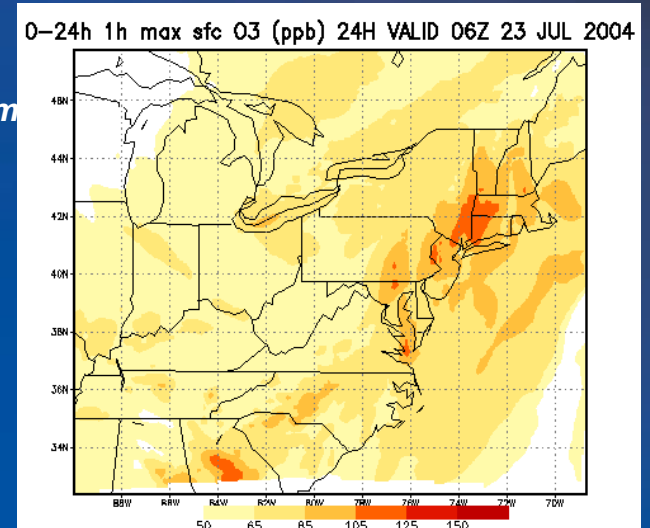
- ✓ Updated Mobile Emissions using MOBILE6 inventory

- ✓ Simplified Temperature dependency on mobile emissions

- **Real-time Verification**

- BUFR  $O_3$  and CMAQ output evaluated

with VSDB/FVS system



# Current Air Quality Forecasting

## *Experimental Expanded Domain Configuration*

- **Eastern US** : 48 hour forecasts of ozone ( $O_3$ ) : 06 and 12 UTC runs

- ✓ **3x expanded domain** (East of Rockies, 268x259x22) run in parallel

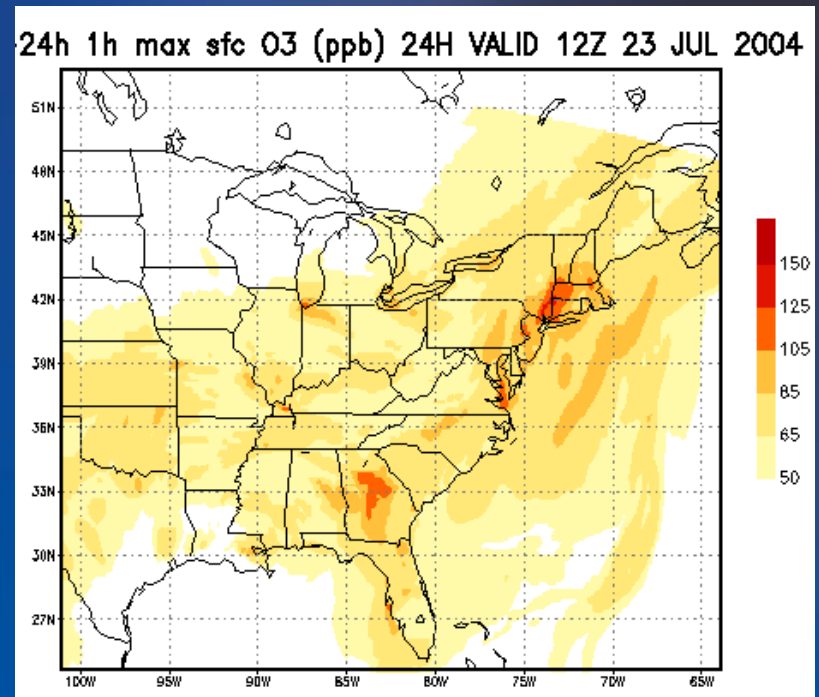
- ✓ Same Configuration as NE US Run except:

- ✓ Convective Cloud Mixing from cloud top = 0

- ✓ **Additional processors (~65) used**

on Production machine

- ✓ 12 z Available by 16:10 UTC



# Current Air Quality Forecasting *Research Aerosol Domain Configuration*

- **Eastern US** : 24 hour forecasts of  $O_3$  & Aerosols:  
12 UTC run only

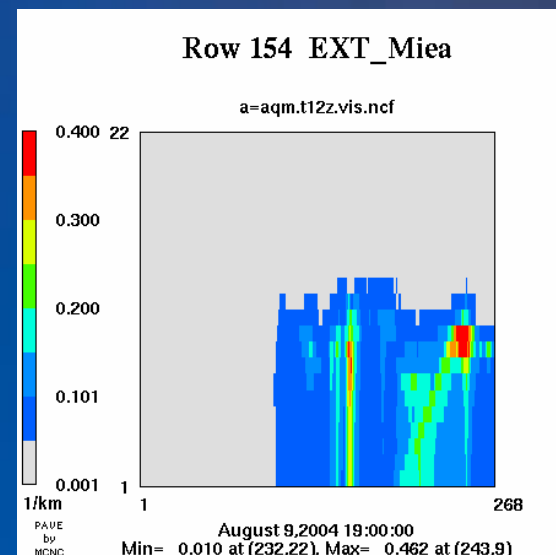
- ✓ Same system as operational except

- ✓ **3x expanded domain** (East of Rockies)  
run

- ✓ **24 hr cycling**

- ✓ **33 processors on Development Machine**  
(less (less reliability, 8x5))

- ✓ Available by 21 UTC



# Current Physics Coupling w/ NCEP NAM



<b>Current Capability</b>	<b>Met Model (Eta, WRF/NMM)</b>	<b>AQ Model (CMAQ)</b>
<b>Core/Dynamics</b>	Rotated Arakawa E grid	Arakawa C Grid
<b>Clouds</b>	Full Ferrier Cloud Microphysics	Eta cloud water for aqueous chemistry
<b>Convective mixing</b>	Betts-Miller Janjic	<i>Entrainment from top turned off</i>
<b>Radiation</b>	GFS*	<i>Derived from Eta RH for photolysis</i>
<b>PBL</b>	Mellor-Yamada TKE	Eta PBL hgt for Pleim-Xiu 1 <sup>st</sup> order K
<b>Land Surface</b>	NOAH common	Eta canopy conductance terms for Pleim-Xiu LSM



# Coupling Developments

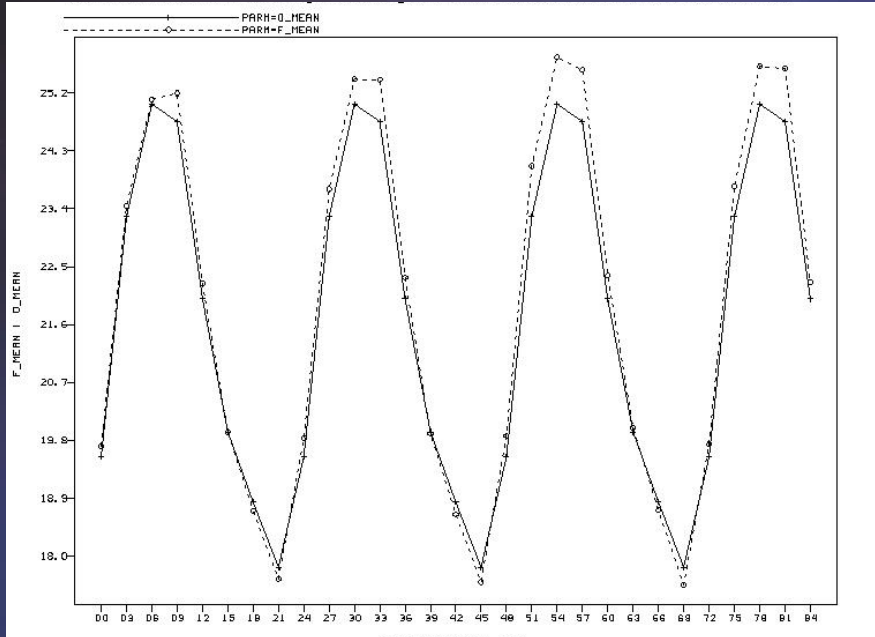


<b>Run</b>	<b>NAM-CMAQ (3x, Conus)</b>	<b>WRF-CMAQ</b>
<b>Domain</b>	Interp to CMAQ C grid	<i>Common Rotated E grid</i>
<b>Vertical Coordinate</b>	Interpolate to CMAQ $\sigma$	<i>Common WRF/NMM <math>\sigma</math>-P</i>
<b>Photolysis</b>	<i>Surface Eta Radiative Scaling</i>	<i>3-D Radiative fluxes</i>
<b>PBL</b>	Eta PBL height into P-X	<i>NAM TKE/Kh to drive mixing</i>
<b>Clouds Aqueous Mixing</b>	Eta cloud water <i>Eta convective cloud base/top</i>	<i>NAM cloud water, graupel &amp; ice Axisymmetric Convective Model (ACM) mixing extended for conv.</i>
<b>LBCs</b>	<i>GFS above 6 km Static below</i>	<i>GFS above 6 km, static below Higher top, improved vertical resolution near tropopause</i>

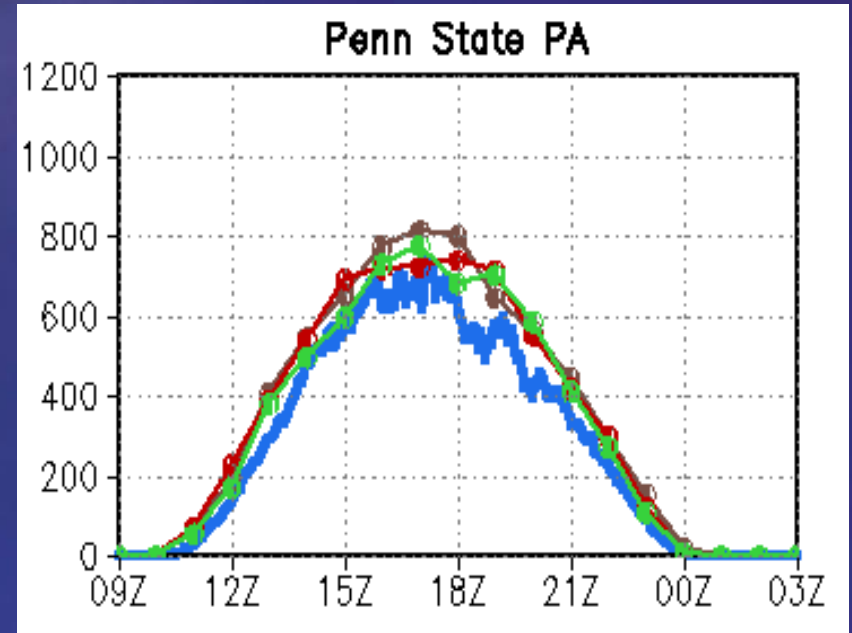


# NAM Verification

## August 2004



Temperature



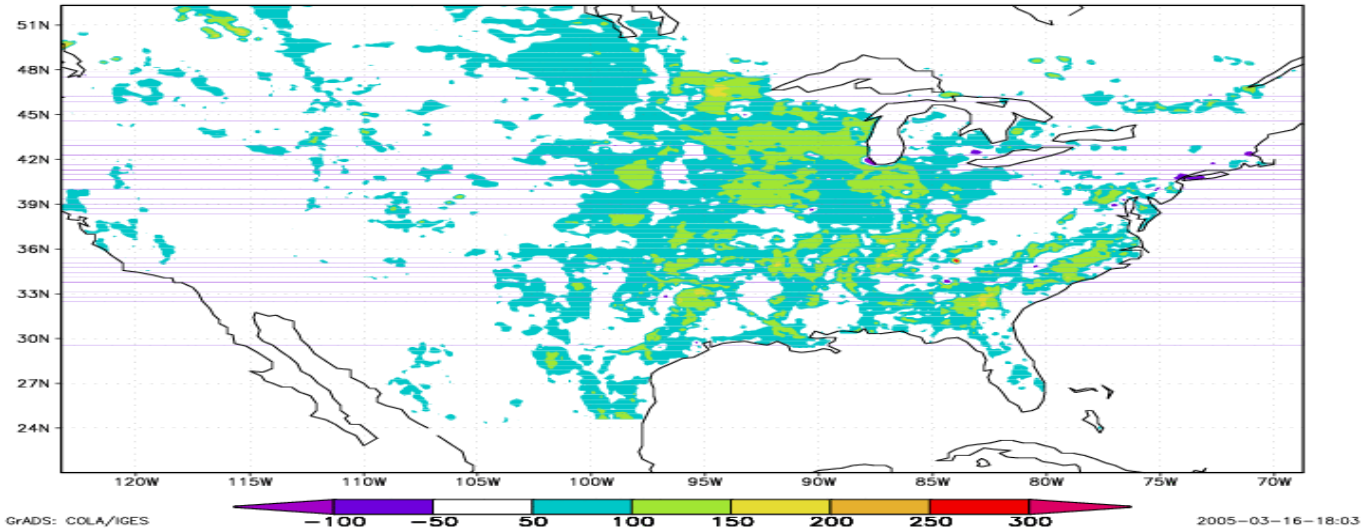
Downward SW





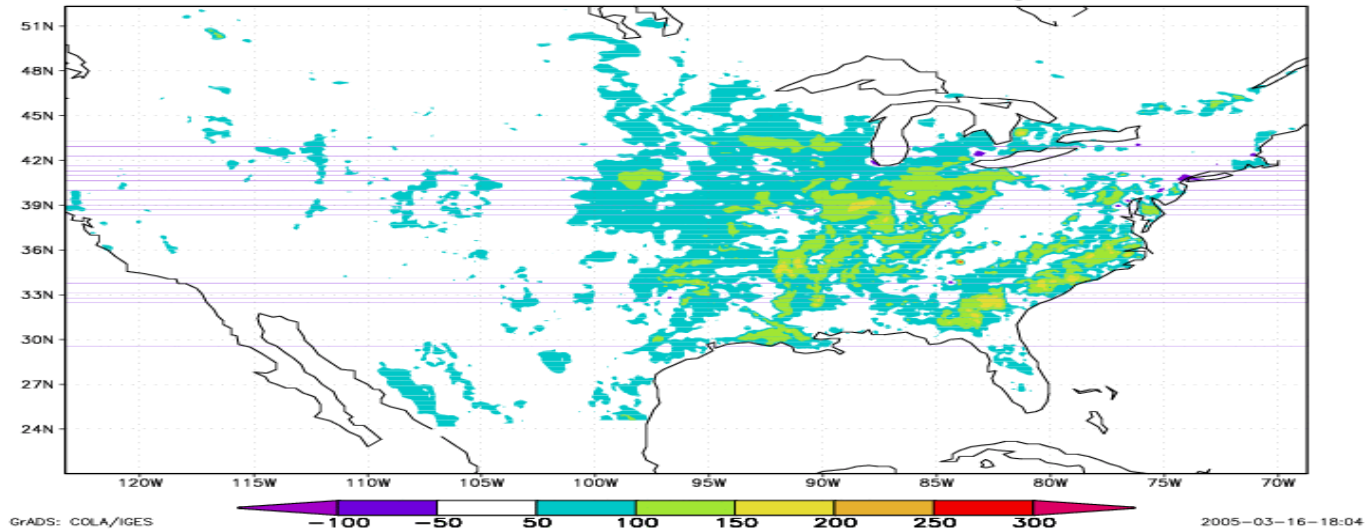
July 16-23

Latent heat flux diff (Eta-Etax) 16-23 Jul 12z+06h



Aug 4-11

Latent heat flux diff (Eta-Etax) 04-11 Aug 12z+06h

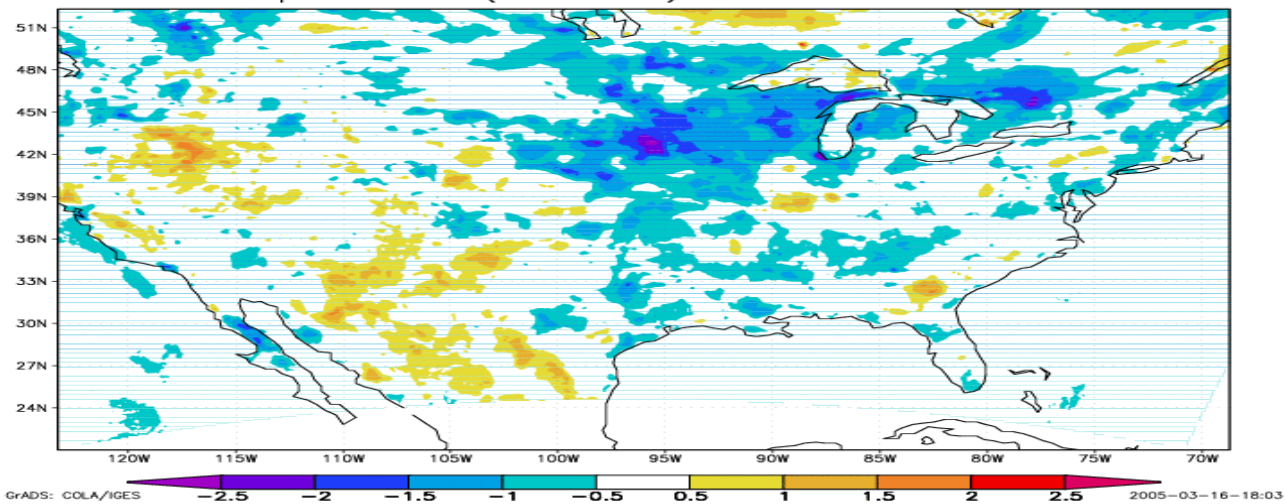




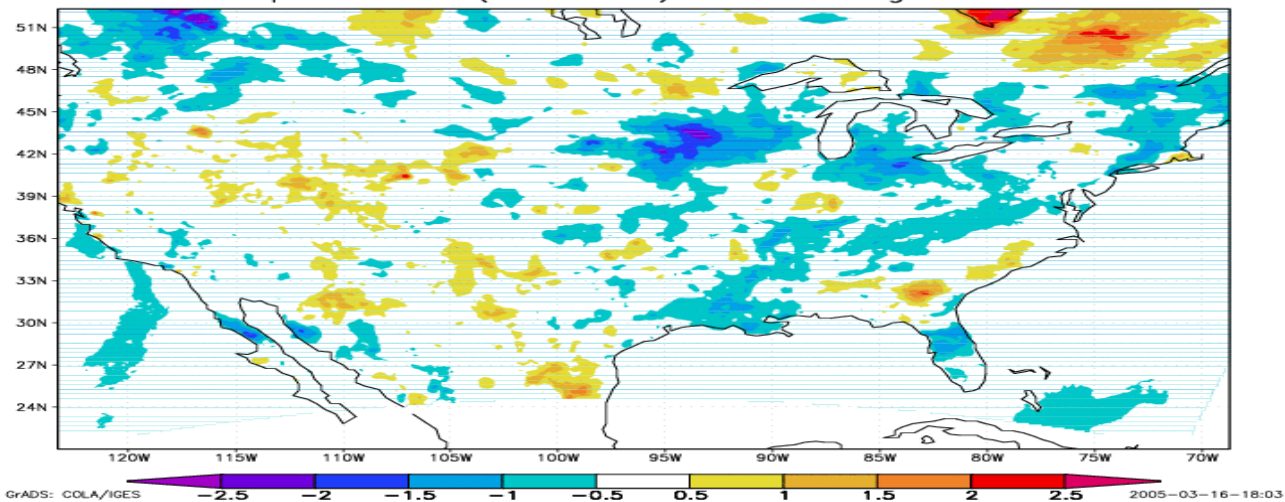
July 16-23



Temp 2m diff (Eta-Etax) 16-23 Jul 12z+06h



Temp 2m diff (Eta-Etax) 04-11 Aug 12z+06h



Aug 4-11



# RETROSPECTIVE TESTING

Runs: P. Lee, M. Tsidulko

Analysis: R. Mathur, D. Kang, J. Pleim,...



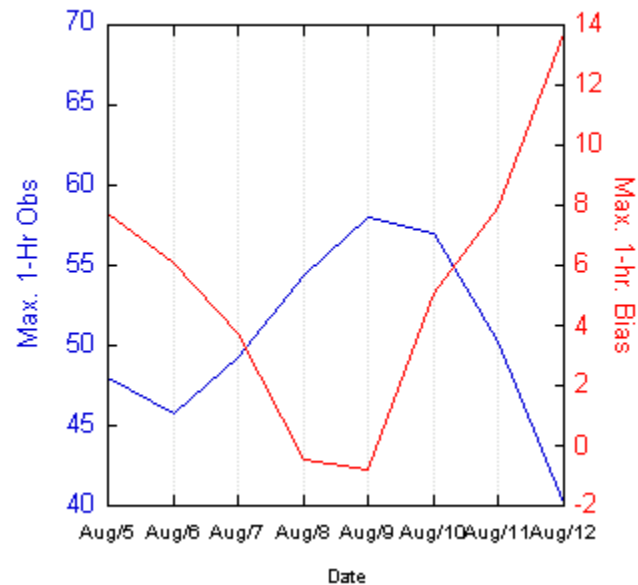
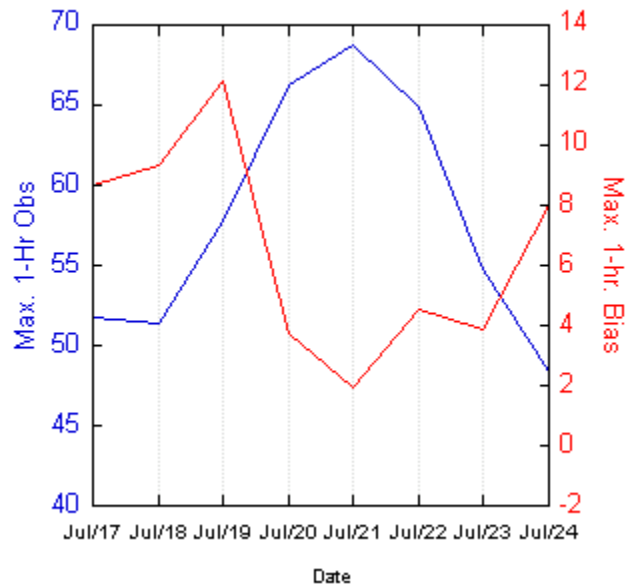
- 2004 Base: 2004 Operational run
- S0: Reflects changes due to Eta-X
- S1: S0 + photolysis attenuation based on Eta radiation fields
- S3: S0 + Mixing from above clouds turned-off
- S5: S1+S3



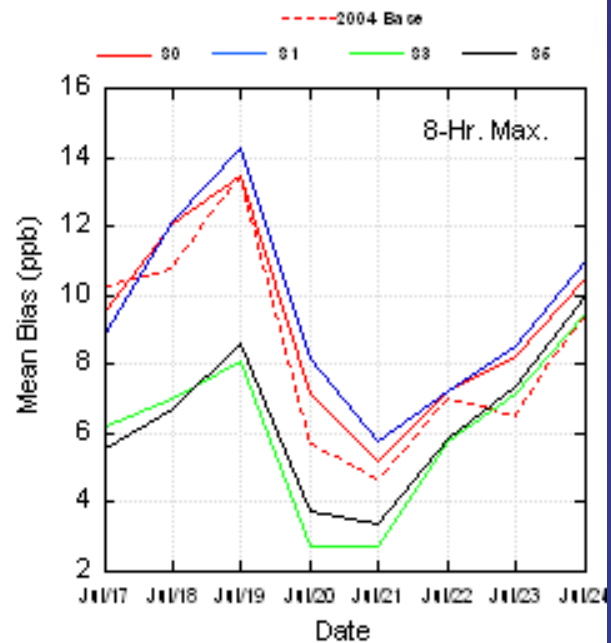
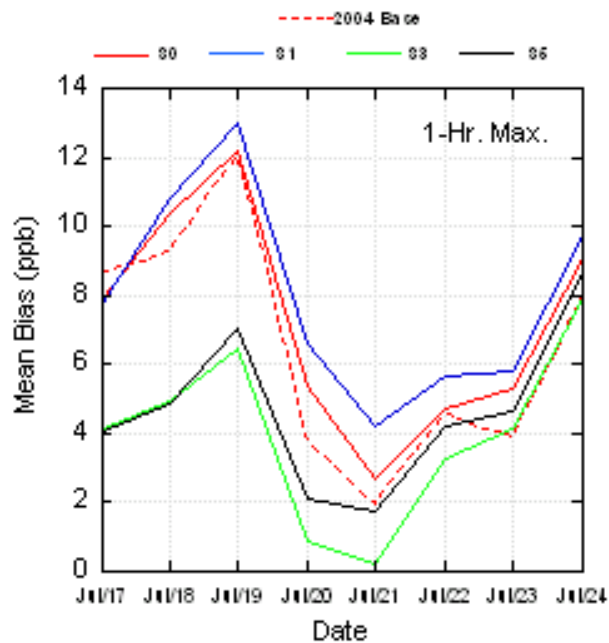
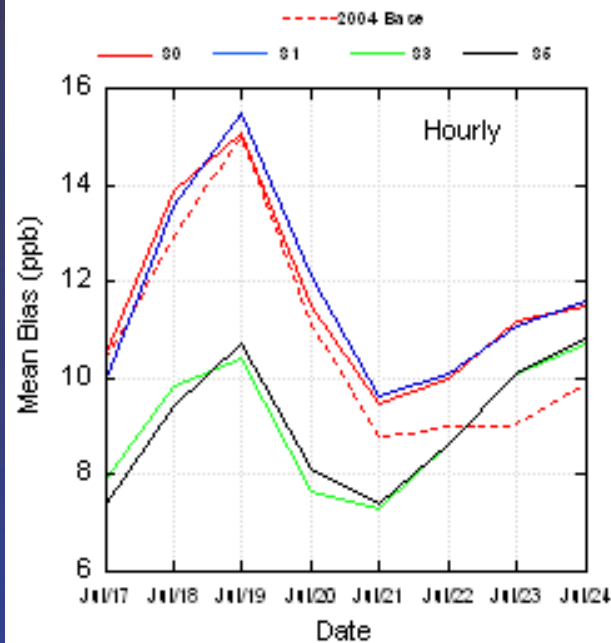
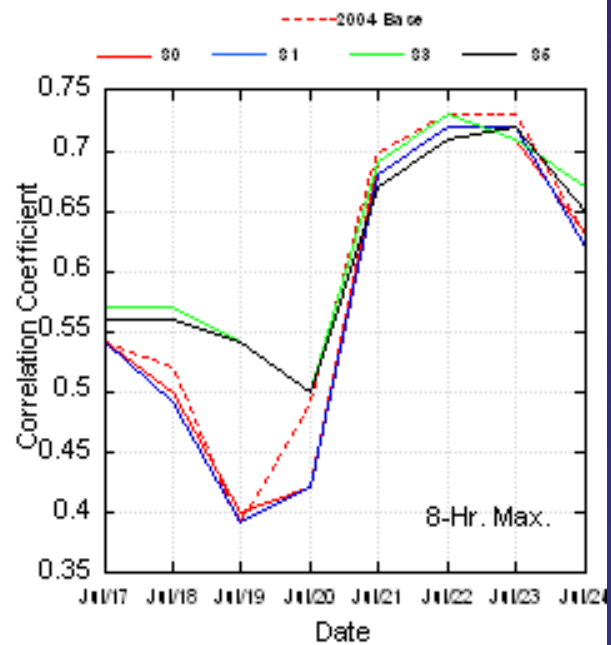
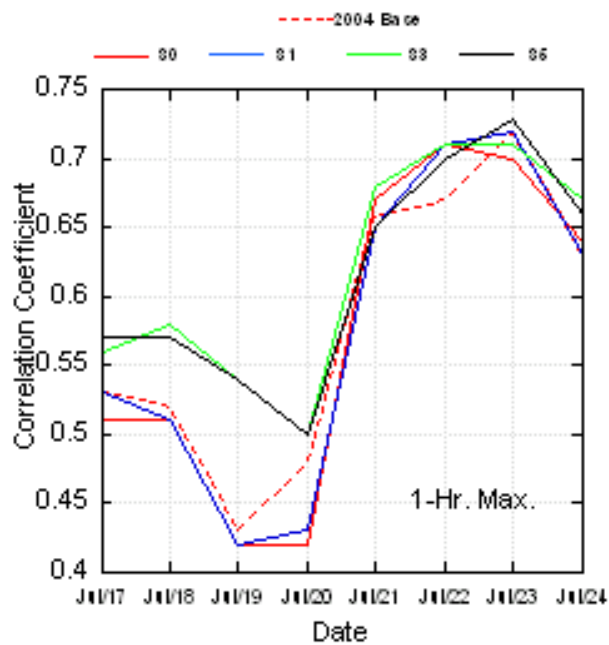
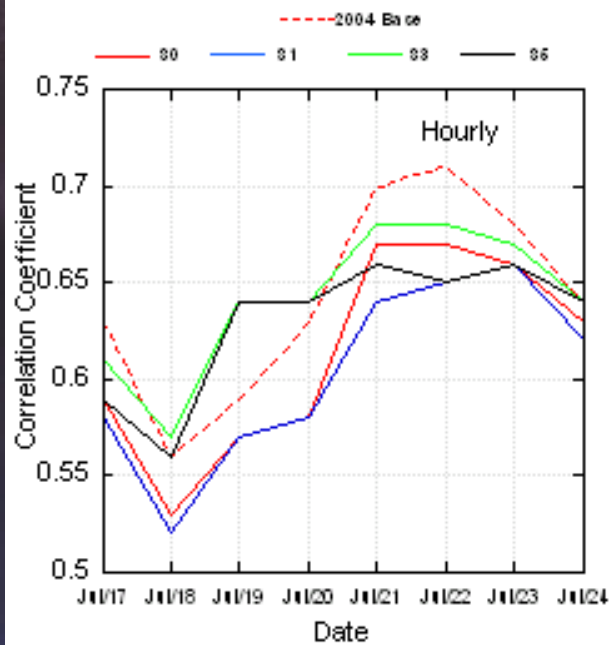
# Analysis Time Periods



- Time Periods
  - 12Z July 16, 2004 – 12Z July 25, 2004
  - 12Z August 4, 2004 – 12Z August 13, 2004
  - 12Z August 8, 2002 – 12Z August 20, 2002



# July Case



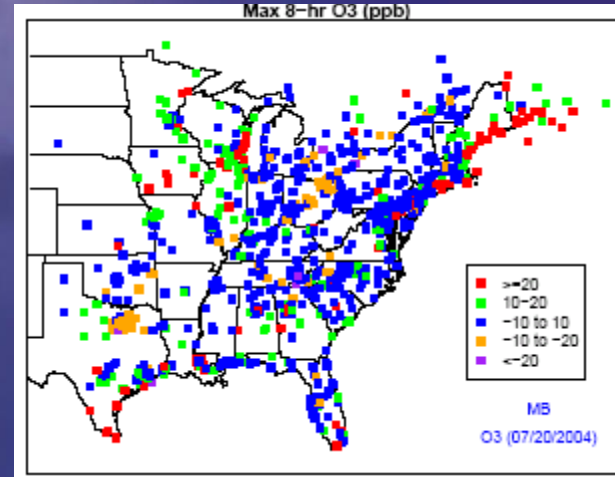
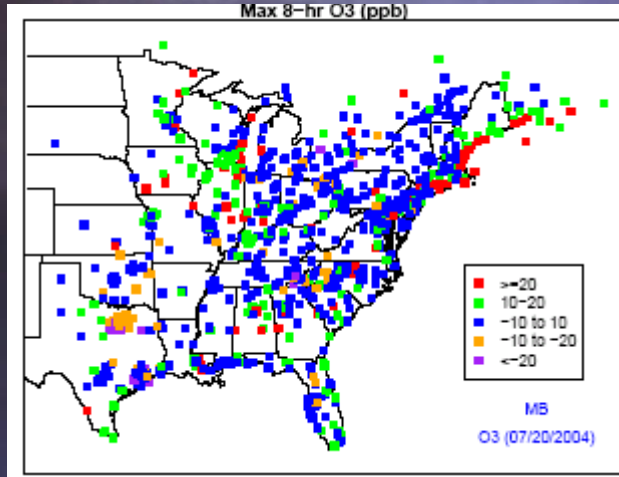


# Max 8-hr O<sub>3</sub> Mean Bias Spatial Distribution: July 21, 2004



2004 Base

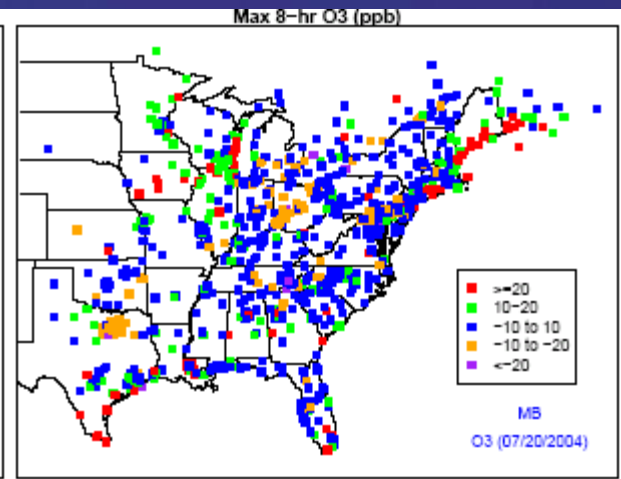
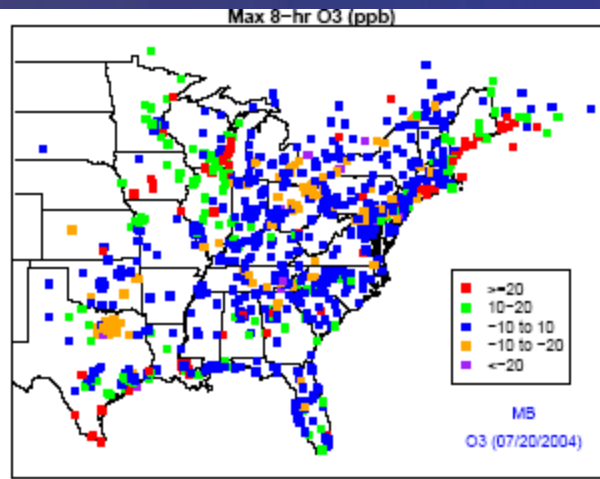
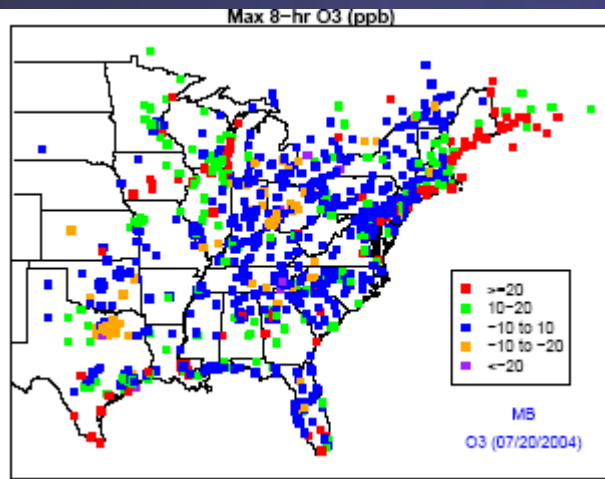
S0



S1

S3

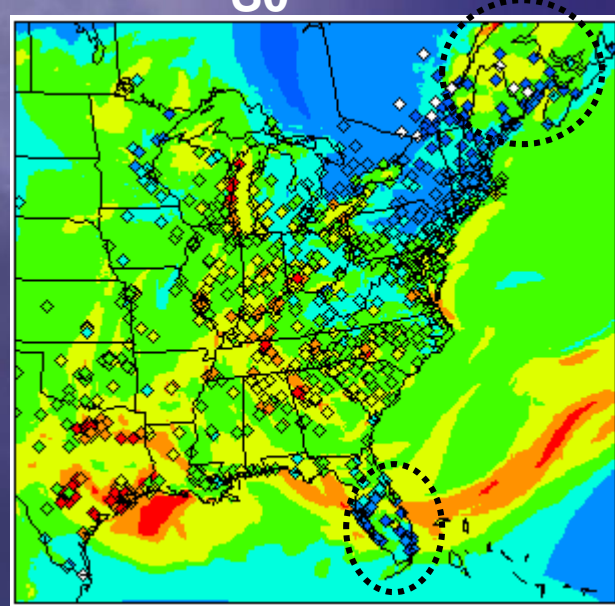
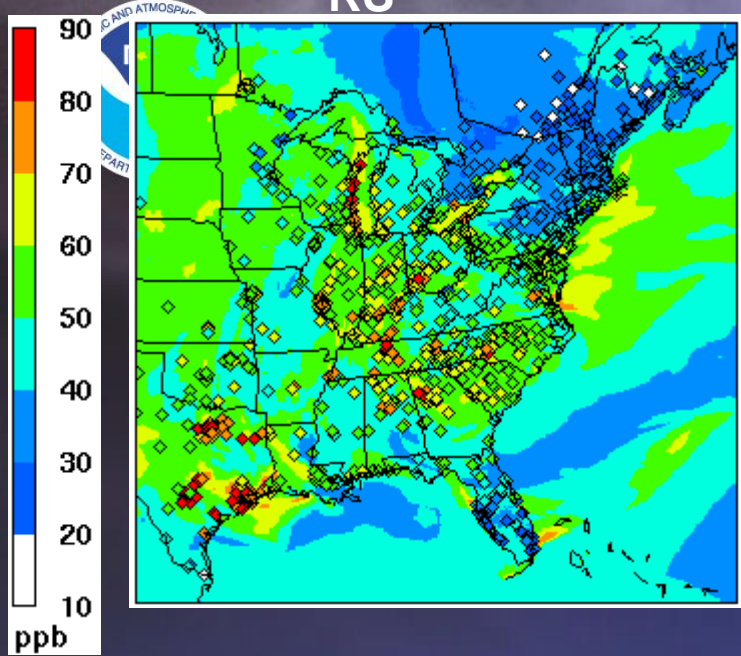
S5





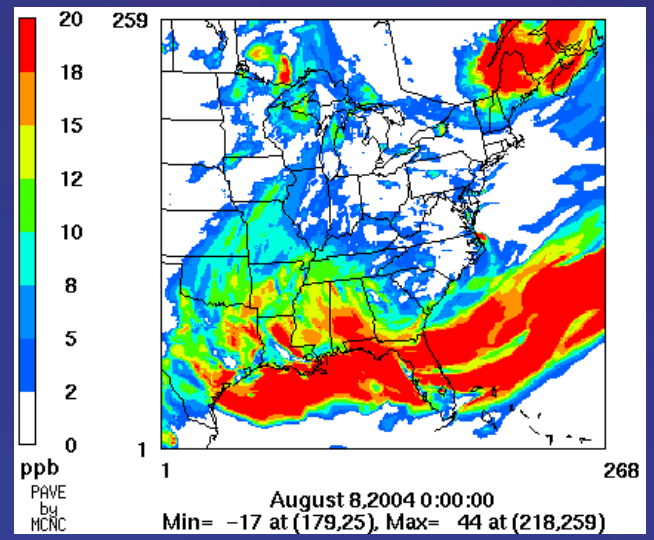
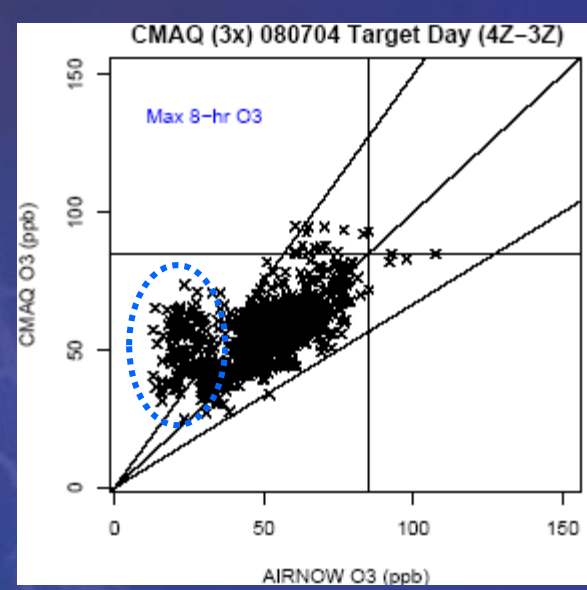
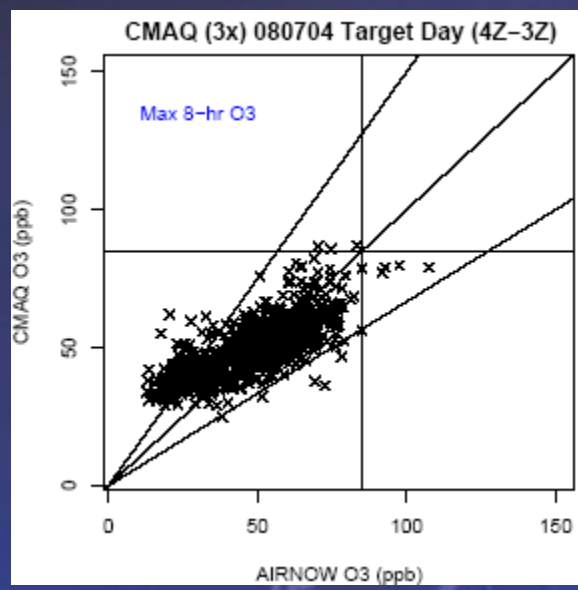
RS

S0



Max. 8-Hr. O<sub>3</sub>  
August 8, 2004

S0-RS



Slight tendency to under-predict

O3 increased regionally,  
Over-predict at low range



# Performance Summary for 2002 Retrospectives

## Comparison of S3 and S4 CMAQ Configuration

**S0:** Reflects changes due to Eta-X

**S1:** S0 + photolysis attenuation based on Eta radiation fields

**S2:** S0 + ACM-type cloud mixing

**S3:** S0 + Mixing from above clouds turned-off

**S4:** S1+S2

**S5:** S1+S3



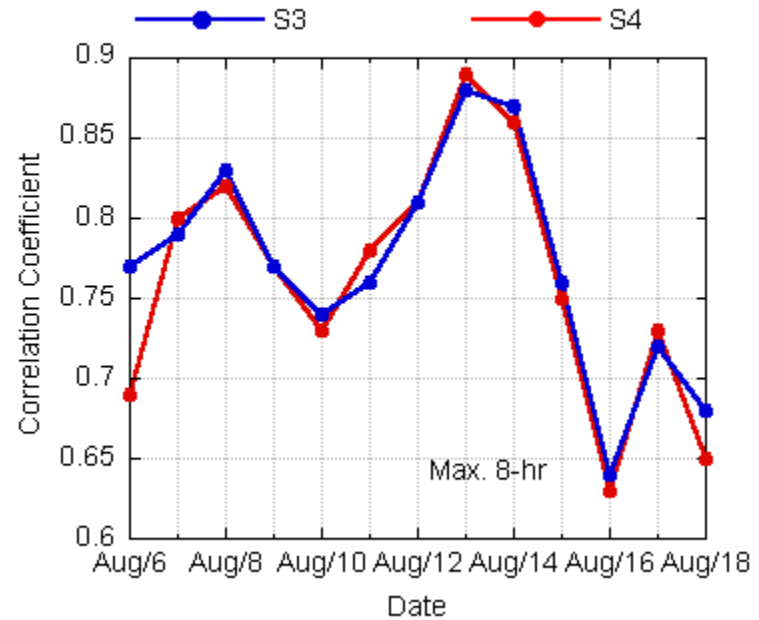
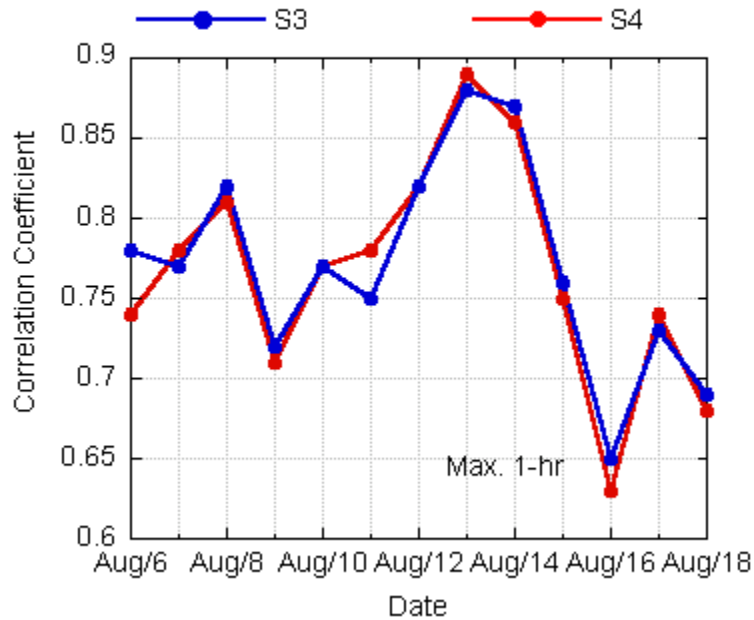


# Performance Summary: August 6-18, 2002



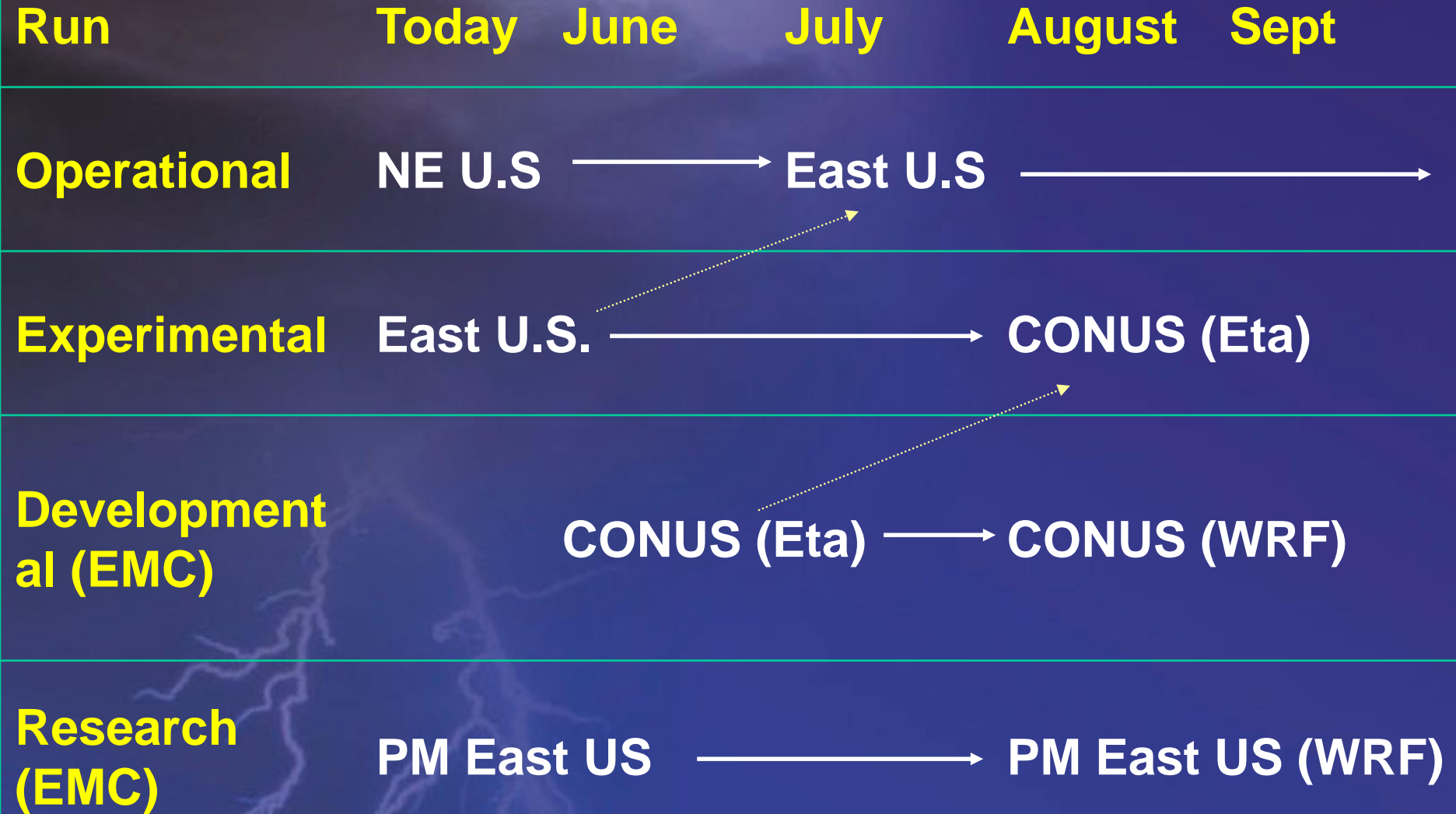
## Max. 1-Hr.

## Max. 8-Hr.





# NCEP AQ Runs





# Developmental Testing

## *WRF-CMAQ (East U.S)*



- **WRF/NMM tests**
  - *Test common vertical Sigma coordinate*
  - *Test common horizontal rotated E grid coordinate*
- **Improved Radiation Coupling for Photolysis**
  - *Sfc and 3d radiative fluxes*
- **Improved Cloud Coupling for cloud mixing & aqueous chemistry**
- **Improved PBL coupling for mixing**
- **Improved Emissions**
- **Improved LBCs**
  - *Improved vertical resolution near tropopause*
  - *Raised CMAQ model top*
- **Full bundle tests**



# Verification Tasks

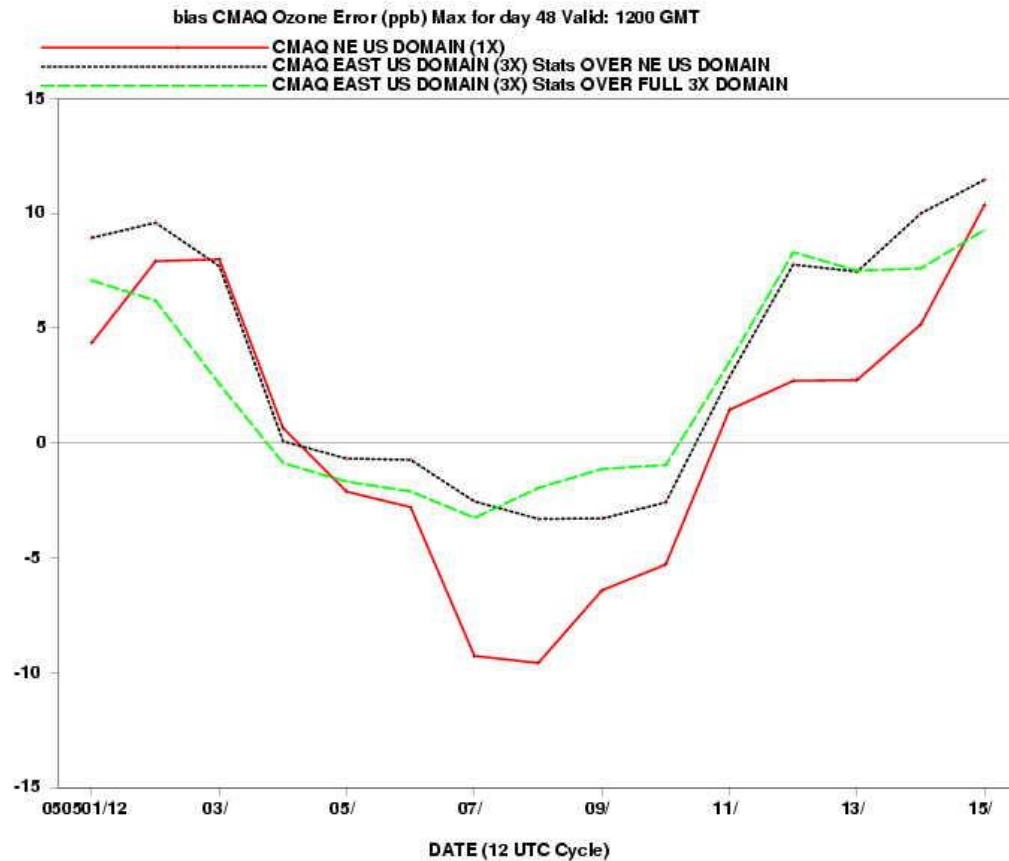
- **Implement near real-time ozone FVS verification system at NCO:**
  - *Statistics for RMSE, Bias, Correlations for full and sub regions*
  - *Contingency stats: Accuracy, POD, FAR, CSI, Threat scores for hrly, 8hrly, daily max*
- **Detailed evaluations of Eta/WRF met. forecasts**
  - *Compare ozone errors with Temperature, RH, winds, PBL height, cloud cover, sfc flux errors*
- **Explore additional mesonets**
  - *Ozone: rural networks(ETOS...)*
  - *Aerosols: AIRNOW, AERONET, IMPROVE, CASTNET?*
  - *Lidars: REALM*
  - *Satellite case studies for CMAQ-aerosols :*
    - **GASP, MODIS, AURA/OMI&TESS**



# FVS O3 Real-Time Verification



## Daily Maximum Ozone Bias





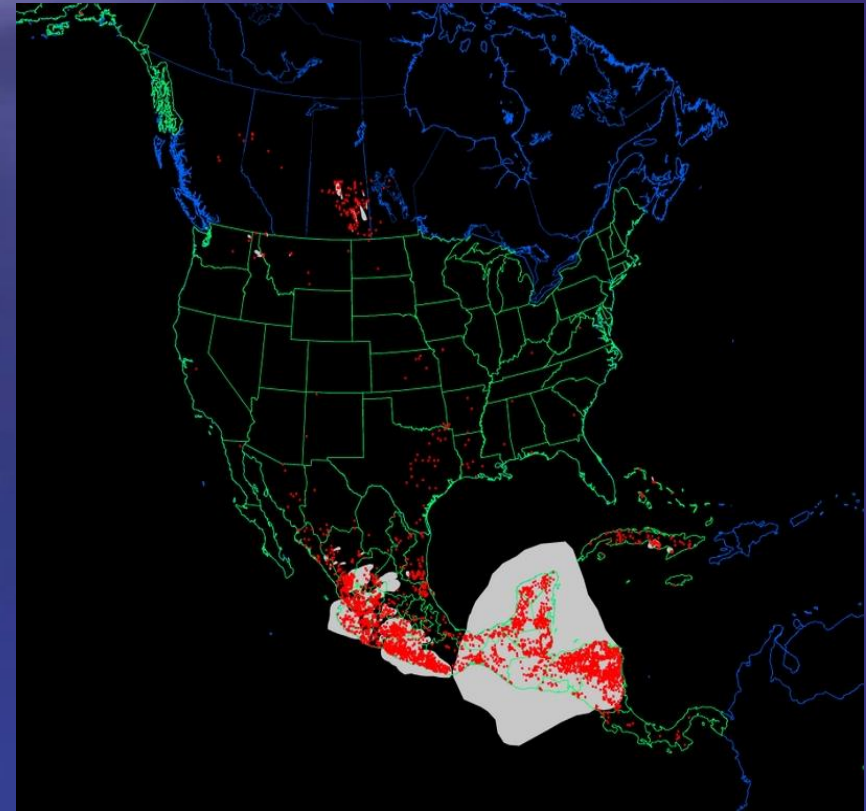
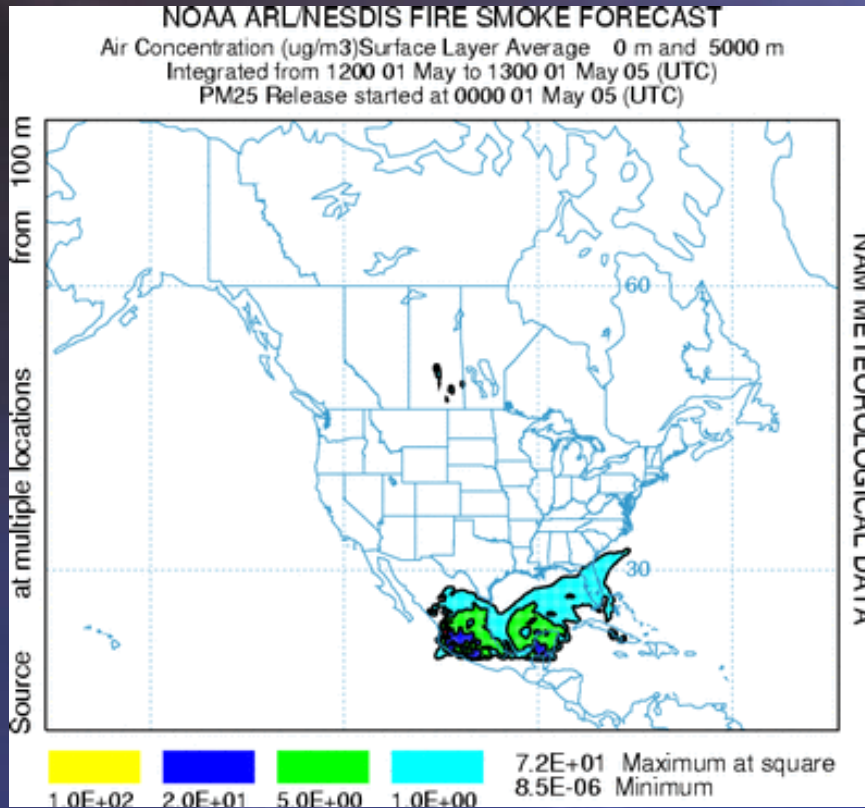
# *Hysplit fire smoke*



- **Jan. 2005**
  - *Upgraded Hysplit for volcanic ash, radiological releases*
  - *web visualization*
- **Sept. 2005**
  - *Hysplit smoke w/ NESDIS HMS source locations retrospective & real-time tests*
  - *USFS smoke emission system (w/o NetCDF)*
  - *Retrospective tests*
  - *Real-time parallel tests*
  - *GASP, MODIS AOD verification performed by NESDIS*



# Hysplit fire smoke verification



1 hr avg PM2.5 conc  
0-5000 m

NESDIS Fire Location and  
Visible Plume



# Data Assimilation/Global System Tasks



- **CMAQ data assimilation:**
  - *Plan for surface ozone assimilation*
  - *Correlate sfc ozone w/ precursors (Nox VOCs)*
- **GFS: Improved chemistry for regional LBCs**
  - **Ozone:**
    - Include tropospheric product/loss rate terms
    - Test reduced ozone chemistry (U.Wisc-RAQMS)
    - Begin testing assimilation of AURA/OMI
    - CMAQ LBC impact studies
  - **Aerosols:**
    - Include NASA-GOCART reduced biomass burning/dust and emission processes
    - Begin testing assimilation of MODIS & AURA/TESS
    - CMAQ LBC impact studies





# Summary



- ***Retrospective and real-time results show improvements***
  - Mean daytime bias reduced from ~17 to 5 ppb
  - Mean daytime rmse reduced from 22.8 to 14.5 ppb
  - However, still general overprediction in day, poorer performance at night,
  - Temporary Fix of over-mixing from downward entrainment of strat(gfs) ozone
- ***FY05 Focus***
  - Improved dynamics/physics coupling
  - Begin assimilation
  - Improve verification



# BACKUPS



# Air Quality Forecasting User Access

## ✓ NE, and East Domain :

- ✓ **Public:** NDGD and TOC ftp server
  - ✓ *Surface ozone predictions*
- ✓ **State Forecasters:** HPC web site
  - ✓ *Sfc O3 & met plots*
  - ✓ *Daily (2pm) conference calls*
  - ✓ *HPC forecasters trained*

## ✓ Experimental Domain (Conus & WRF O3):

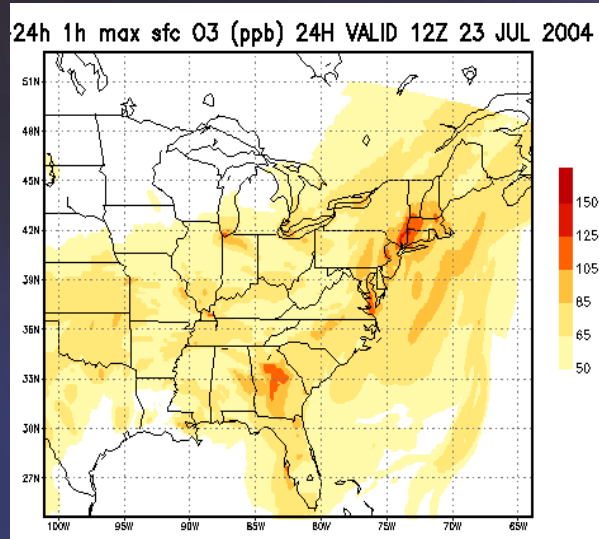
- ✓ **Focus group:** EMC web site
  - ✓ *Expanded met plots (pbl hgt, sw rad, ventilation index....)*
  - ✓ *Sfc & upper level O3 and precursor plots (NOx, NOy,CO,SO2)*

## ✓ Research (Aerosols)

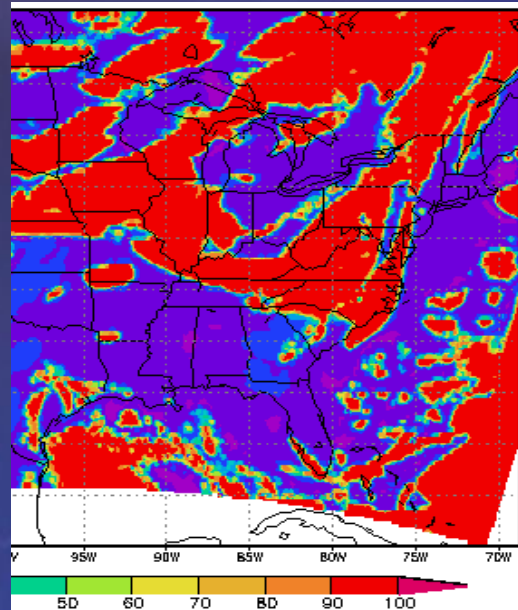
- ✓ **Sfc PM, AOT**



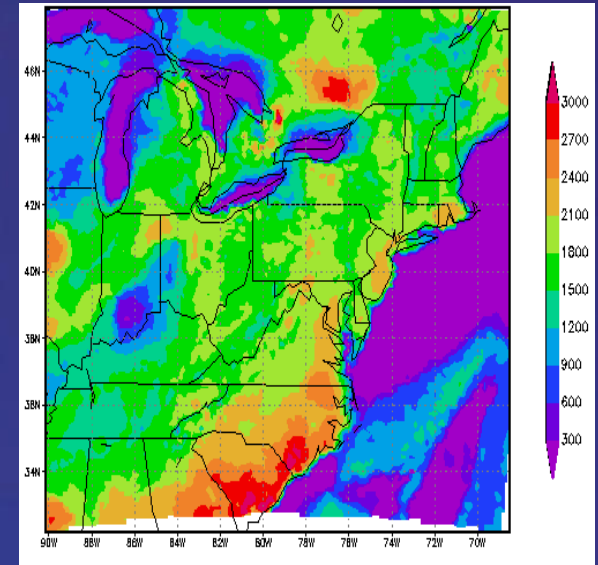
# NCEP Graphical Products



Predicted Sfc Ozone  
(1, 8h, max)



Eta cloud cover



Eta PBL hgt



# Potential short-term collaboration projects



- Evaluation of NCEP WRF-CMAQ ozone & aerosol simulations
  - *Experimental & rural obs networks (eg: ETOS, AERONET, REALM lidar network)*
  - *GOES/MODIS satellite evaluation*
- Assimilation of AIRNOW ozone data into CMAQ initial conditions
- Improved cloud mixing, aqueous chemistry PBL coupling with WRF-CMAQ
- Testing of WRF-Chem on-line system to offline WRF-CMAQ forecasts

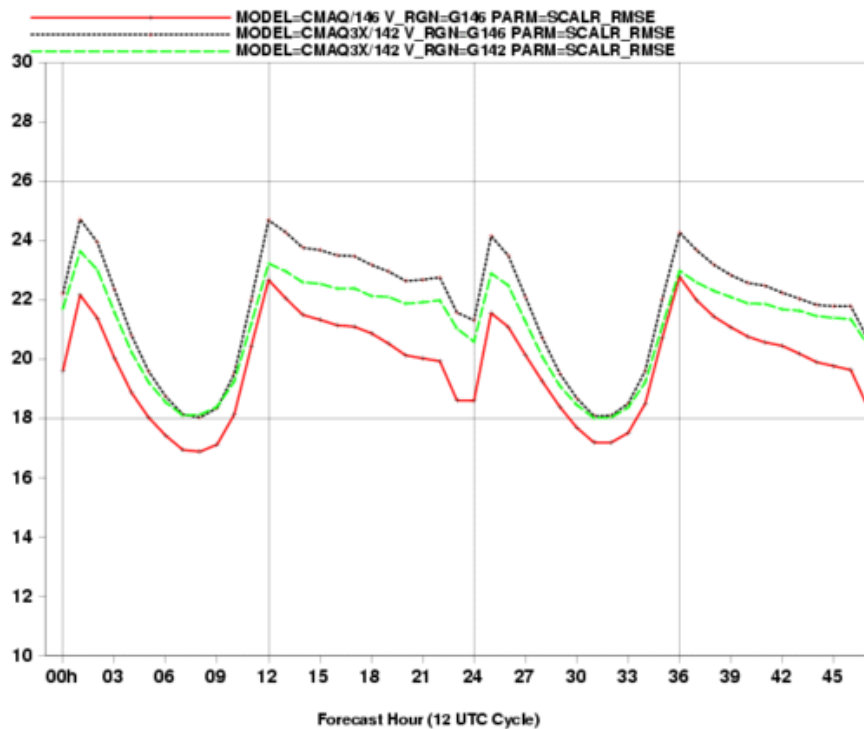


# Real-Time Verification

## *EMC FVS time-series binned by FHR*

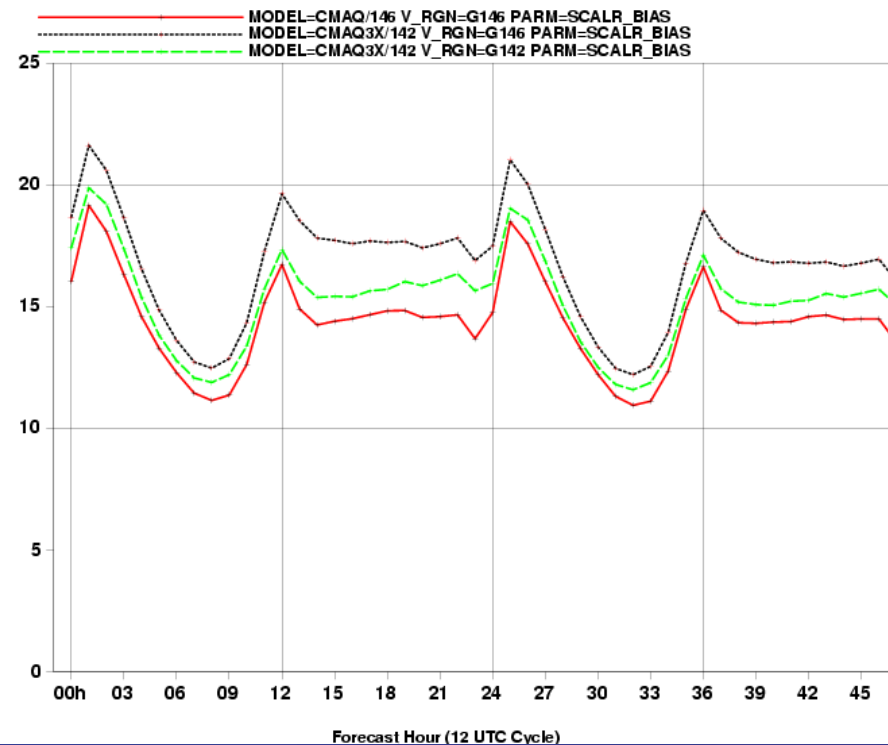


rms CMAQ Ozone Error(ppb)averaged by forecast hour for all fcsts thru 20040915



RMSE

bias CMAQ Ozone Error(ppb)averaged by forecast hour for all fcsts thru 20040915



Bias

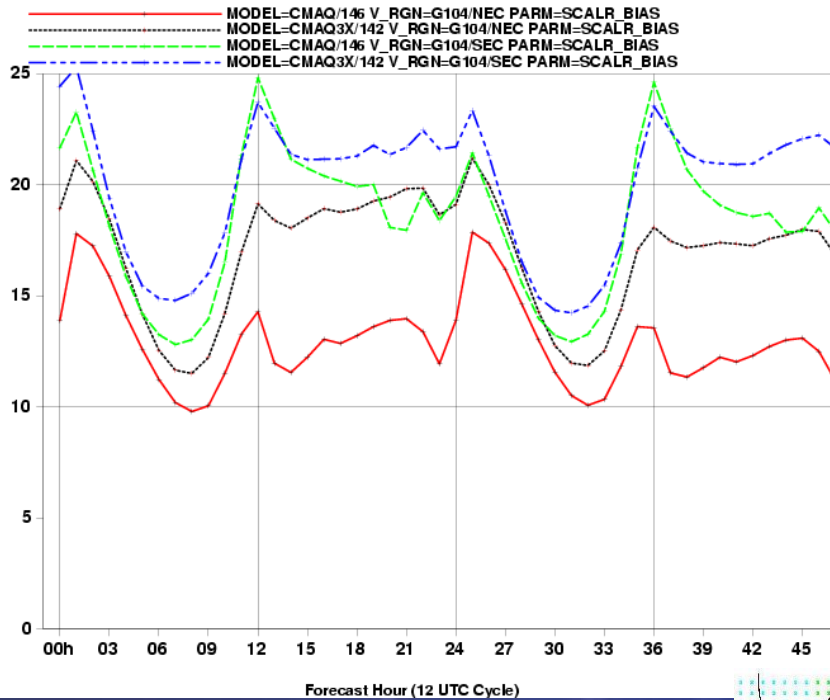


# Real-Time Verification

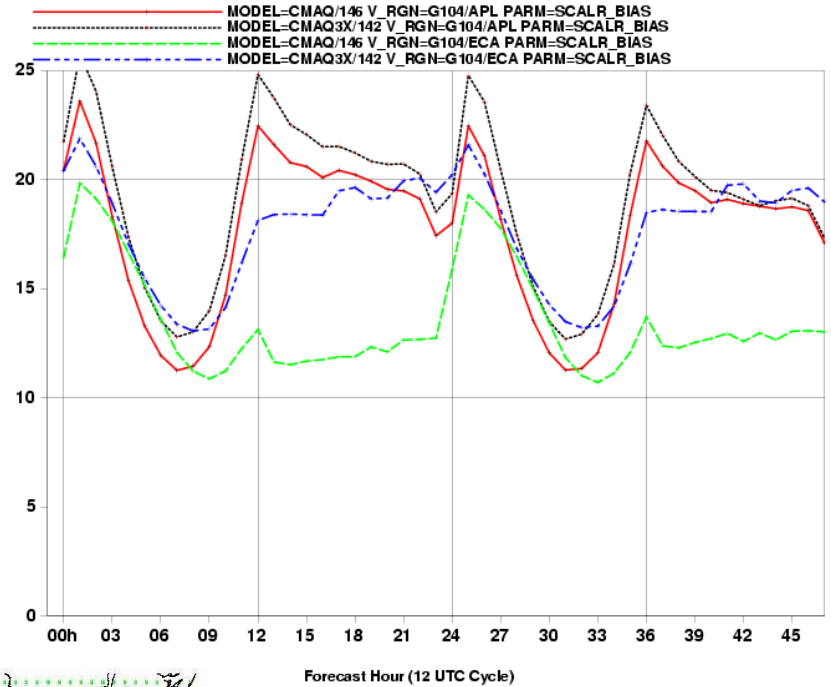
## EMC FVS forecast by sub-region



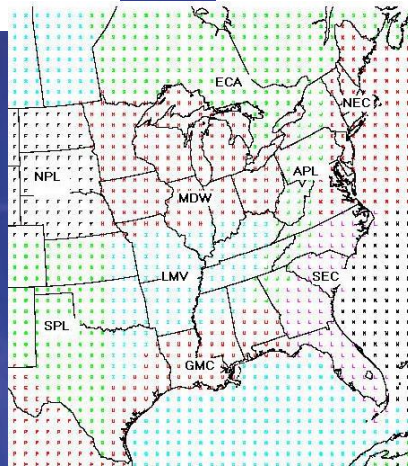
CMAQ Ozone Error(ppb)averaged by forecast hour for all fcsts thru 20040915



s CMAQ Ozone Error(ppb)averaged by forecast hour for all fcsts thru 20040915



BIAS 1x vs 3x  
NE, SE US



BIAS 1x vs 3x  
E. Canada, APL US



# Retrospective Tests

## *Eta-CMAQ (East U.S)*



- Upgraded Eta Met. Driver tests (S0)
  - *1 km NOAA Landuse, soils*
  - *Improved cloud-radiation effects*
  - *2 mb top, improved precip assimilation*
- Improved Radiation Coupling for Photolysis (S2)
  - *Sfc radiation flux scaling*
- Improved Cloud Coupling for cloud mixing *and aqueous chemistry?*
  - *Use graupal, ice fields for aqueous*
  - *Use convective cloud base/top for mixing*
- Improved PBL coupling for mixing
  - *Use 3-D TKE Kh fields*
- Improved Emissions
- Improved LBCs
- Full bundle tests
- Begin Real-time Parallels





# Operational Requirements



Driven by NCEP Operational Meteorological Model (Eta-12 and WRF/NMM)

- **I/O Formats:**
  - *Only machine binary, GRIB and BUFR, disk space limitations*
- **Time Requirement:**
  - *12 Z 48 hour forecast available by 17:25 Z (1:25 pm EDT)*
  - *06 Z 48 hour forecast available by 13:00 Z ( 9 am EDT)*
  - *65 IBM Power 4 procs available*
  - *12 Z start after Eta is complete (14:30 Z)*
- **Robustness:**
  - *Thoroughly tested & evaluated with retrospective and real-time experimental runs*
  - *Available to NWS Gateway, NDGD: 99% reliability, 24x7 NCEP support*
  - *Accuracy: 90% exceedence hit rate*



# Summer 05 Planned NCEP Runs



Run	To EMC	To NCO	Real-time runs
Operational (3x East U.S.)	2/1/05	3/15/05	5/1/05
Experimental (CONUS U.S.)	3/15/05	5/1/05	6/1/05
Developmental (CONUS-WRF)	6/1/05 <i>If WRF/NMM is running realtime</i>	7/15/05	9/15/05
Research (Aerosols)	Real-time: Winter 05  Retrospect: Summer 05		
Fire Smoke (Hysplit-I)	12/31/04	2/1/05	3/1/05
Bluesky-hysplit-II	3/1/05	5/15/05	7/1/05

# Air Quality Forecasting 2004 Verification (1x and 3x)

## ✓ NCEP EMC FVS System :

- ✓ 1 and 8 hour O3 averages
- ✓ **RMSE, Bias, STD, correlation coefficients Time series by fhr and day, subregion**
  - ✓ *using EPA AIRNOW O3 network began 7/12/04*
- ✓ FHO contingency exceedence stats (POD, FAR, threat scores)
  - ✓ *Began 8/1/04*

## ✓ NWS/MDL

- ✓ Daily Spatial obs vs predicted exceedence maps
- ✓ Contingency exceedence stats since June 1

## ✓ NOAA/OAR/EPA

- ✓ Retrospective evaluations (8/12-19, 2003)
- ✓ RT: Similar Stats except stations averaged over CMAQ grid points

## ✓ ICARRT web page: sfc & UL ozone timeseries vs observations



# Implementation Tasks

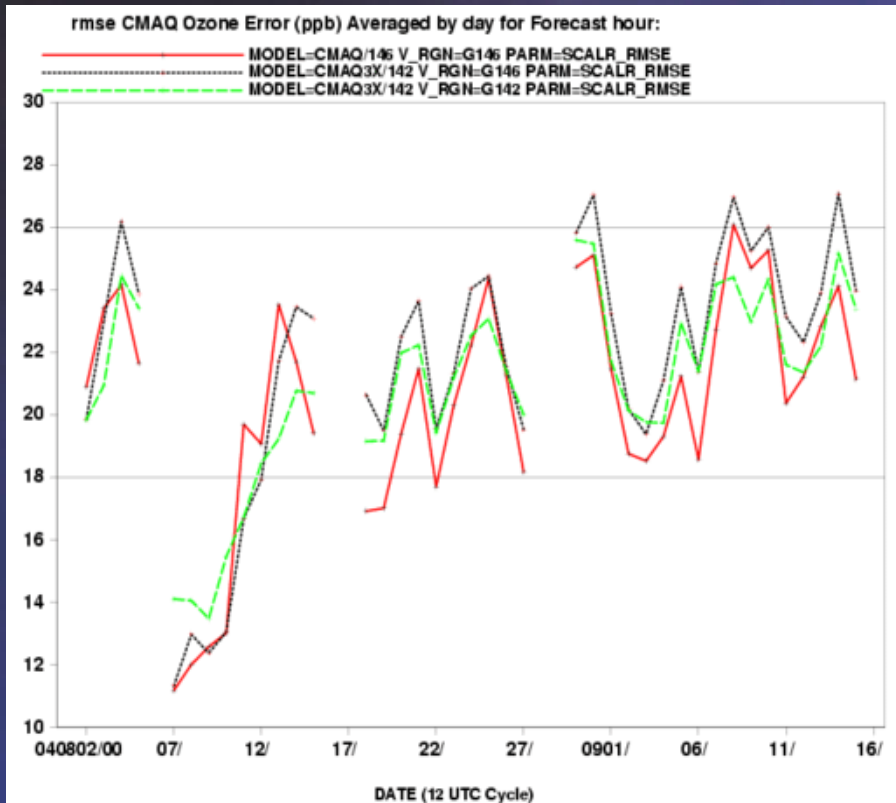


- **Transfer parallel experimental system to Operations:**
  - **Complete agreed upon Charter w/ NCO**
  - **Provide additional Eta/WRF fields from Postprocessors**
  - \* **Transfer upgraded CMAQ to EMC**
  - **Add internal documentation, refine scripts, adjust IO & dataset names**
  - **Support GRIB2 hrly gridded outputs**
  - **Perform 2002/2004 retrospective tests w/ upgraded Eta or WRF**
  - **Perform real-time parallels w/ updated emissions files**
  - **System evaluation against AIRNOW w NCEP FVS**
  - **Prepare estimates of cpu/disk resources for NCO**
  - **Prepare Job Implementation Form (JIFs) requests to NCO:**
    - **Send out Change Notices, update web page change logs**
- **Maintain/improve operational graphics, verification plot web pages**
  - **May require additional output to GRIB files**

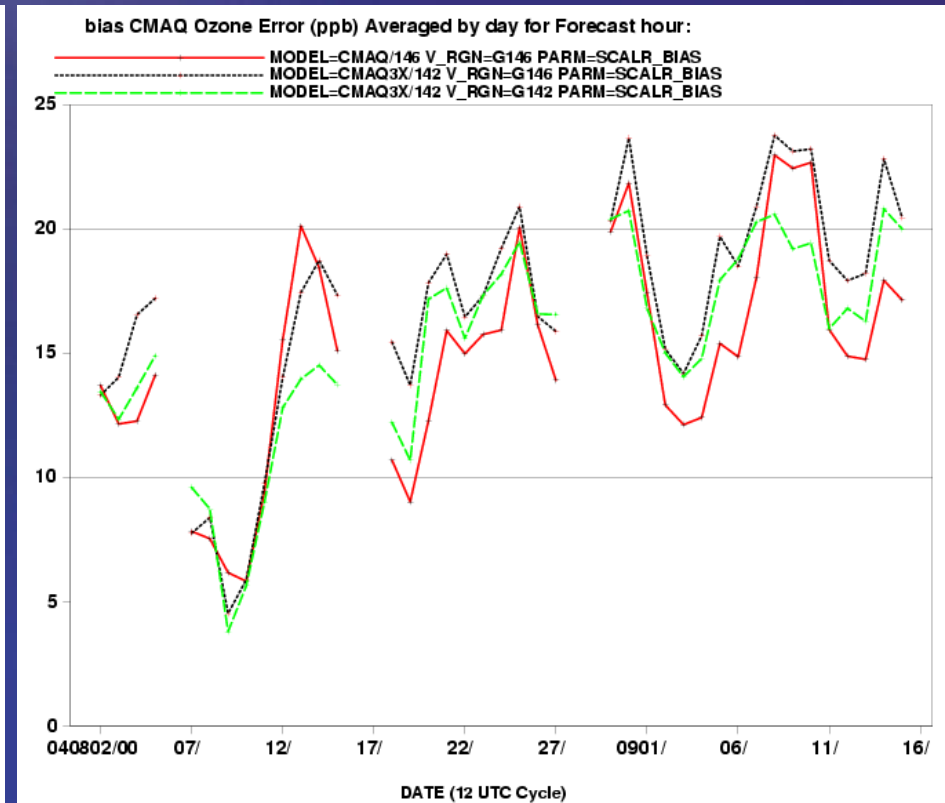


# Real-Time Verification

## *EMC FVS 36 h forecast time-series by day*

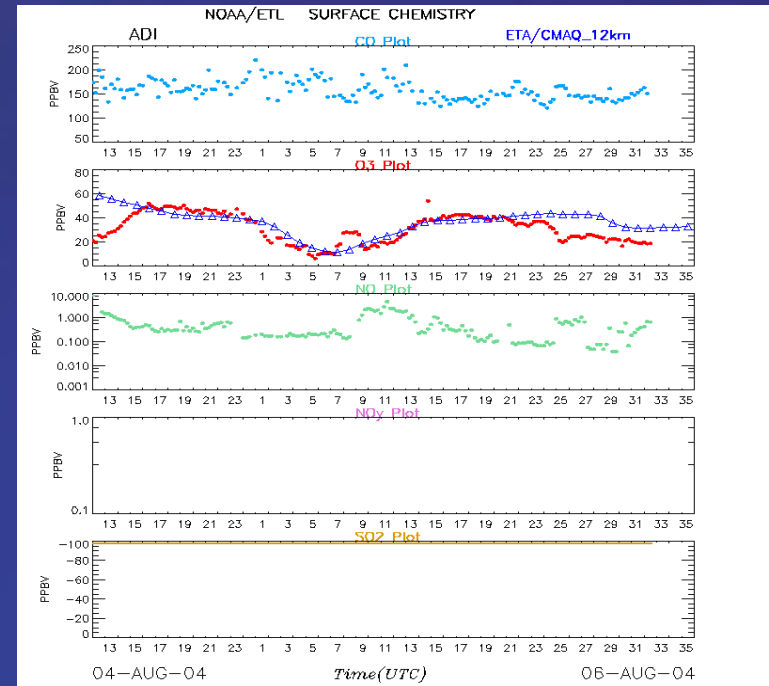
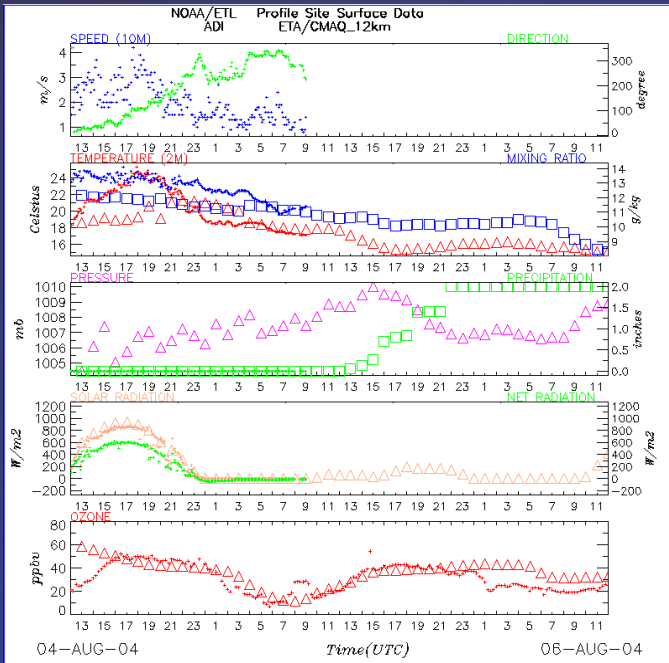
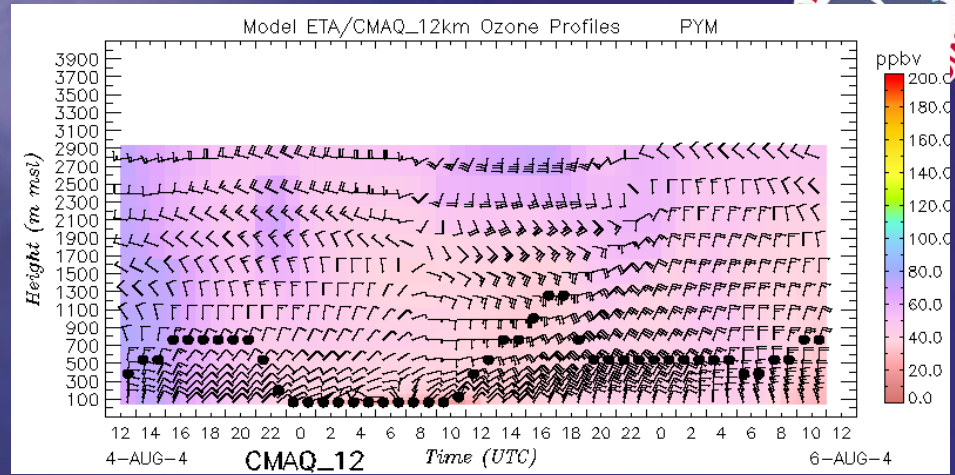
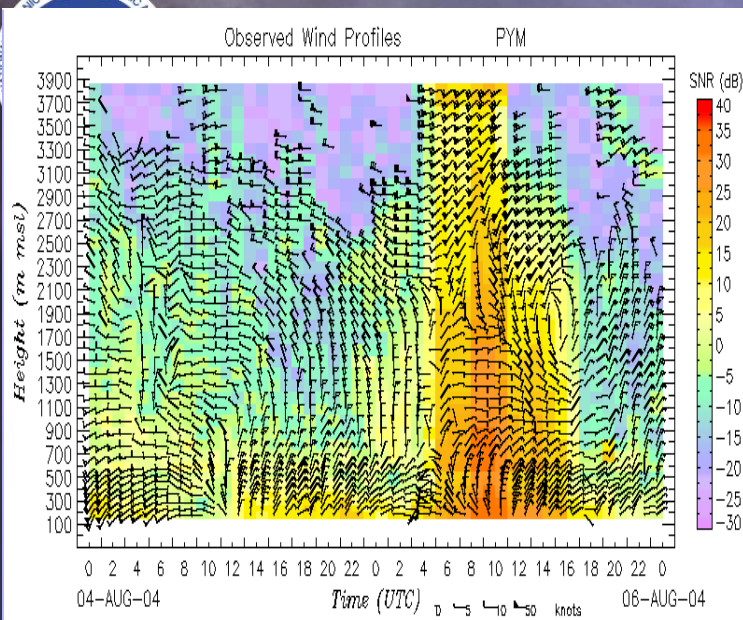
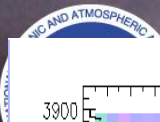


RMSE



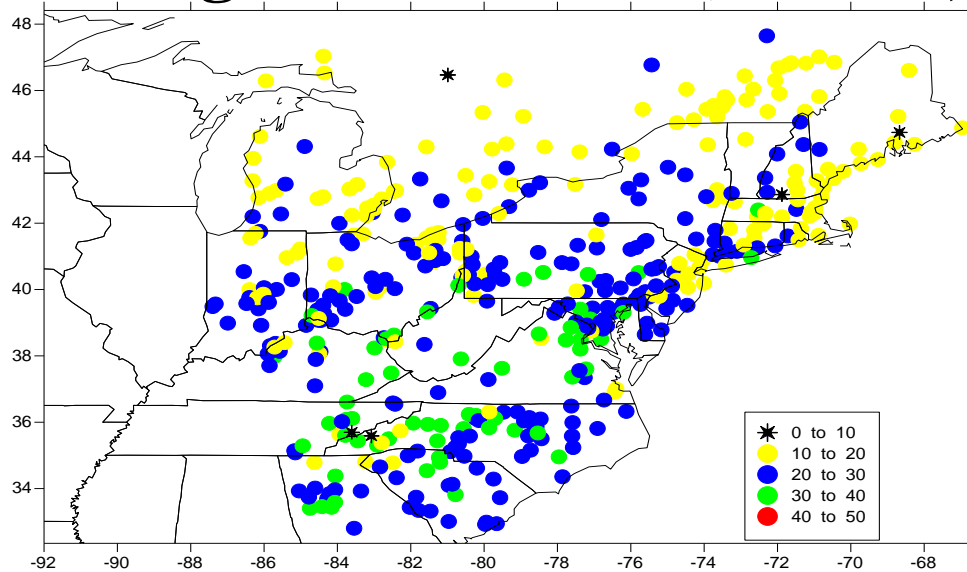
Bias

# ICARRT Evaluation

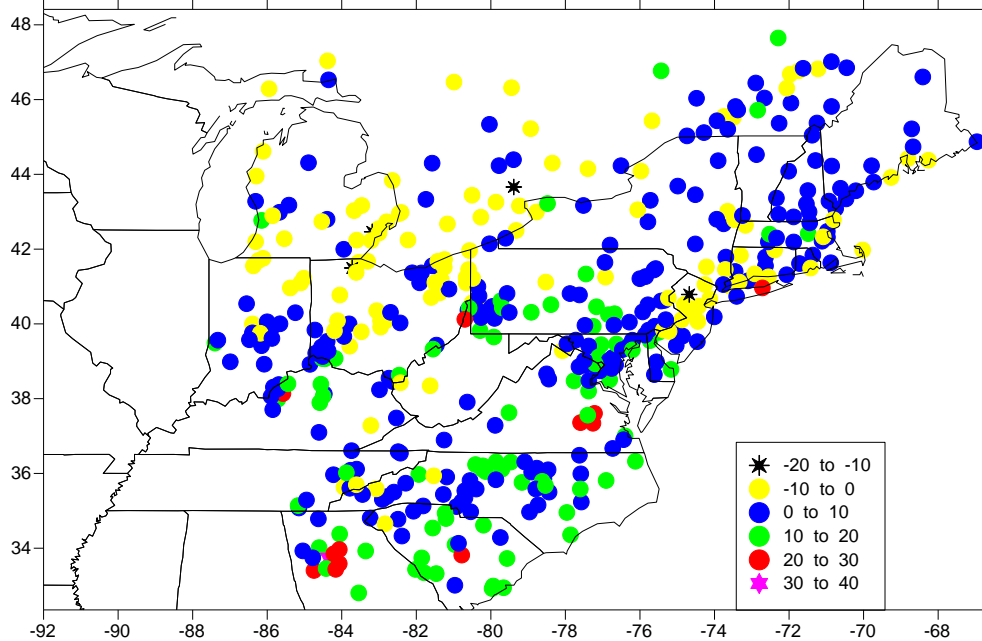


# NE DOMAIN Retros. Evaluation

## 1 Hr Avg ozone Errors (8/12-19, 2003)



RMSE



Mean Bias



# Real-Time Verification

## NWS MDL Evaluation

Predicted vs Obs Exceedence

