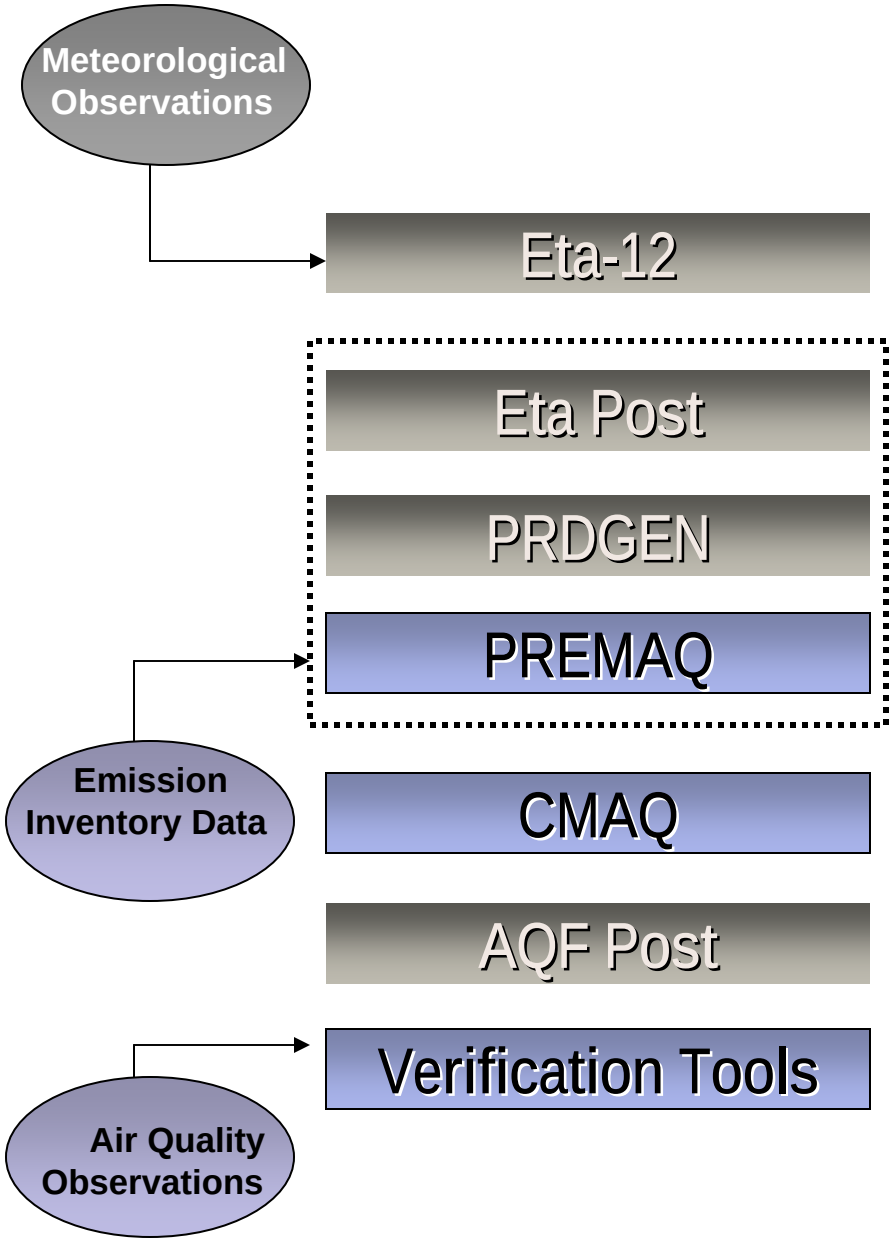
THE COMMUNITY MULTISCALE AIR QUALITY (CMAQ) MODEL:
Model Configuration and Enhancements for 2005 Air Quality Forecasting

Rohit Mathur, Jonathan Pleim, Kenneth Schere, George Pouliot
Jeffrey Young, Tanya Otte
Atmospheric Sciences Modeling Division
ARL/NOAA
NERL/U.S. EPA

Daiwen Kang, Shaocai Yu, Hsin-Mu Lin
Science and Technology Corporation

Eta-CMAQ AQF System



NOAA's Meteorology model

Vertical interpolation from eta to sigma

Horizontal interpolation to Lambert grid

CMAQ-ready meteorology and emissions
(Optimization reduced run-time by half)

EPA's Air Quality model

Gridded ozone files for users

Performance feedback for users/developers

Emission Processing

- Emission Processing is a component of PREMAQ (pre-processor to CMAQ)
- Point Source and Biogenic Source processing from SMOKE
- Area Sources (no meteorological modulation) computed in SMOKE outside of PREMAQ
- Mobile Sources (nonlinear least squares approximation to SMOKE/Mobile6)

Area and Biogenic Sources

- Area Sources: 2001 NEI version 3 inventory used. (CAIR) No changes made to inventory. Computed outside of PREMAQ
- Biogenic Sources: BEIS3.12 included directly into PREMAQ.
- Canadian Inventory: 1995 used (no changes)
- Mexican Inventory: BRAVO 1999 used for point sources (3x domain only)

Mobile Sources

- SMOKE/MOBILE6 not efficient for real-time forecasting
- SMOKE/MOBILE6 used to create retrospective emissions for AQF grid
  - 2005 (projected from 2001) VMT data used for input to Mobile 6
  - 2005 Vehicle Fleet used for input to Mobile 6

Mobile Sources

- Regression applied at each grid cell at each hour of the week for each species to create temperature/emission relationship
- Mobile Source emissions calculated in real-time using this derived temperature/emission relationship

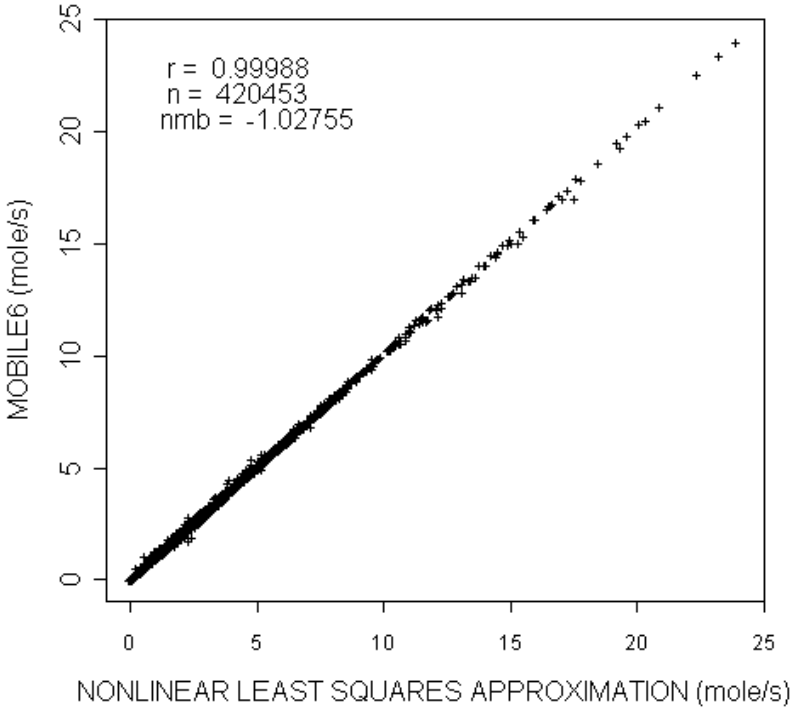
$$Emis_{i,j,t,s} = \alpha_{i,j,t,s}(T_{i,j,t} - T_0)^2 + \beta_{i,j,t,s}(T_{i,j,t} - T_0) + \gamma_{i,j,t,s}$$

- For California used 2001 mobile estimates from CARB

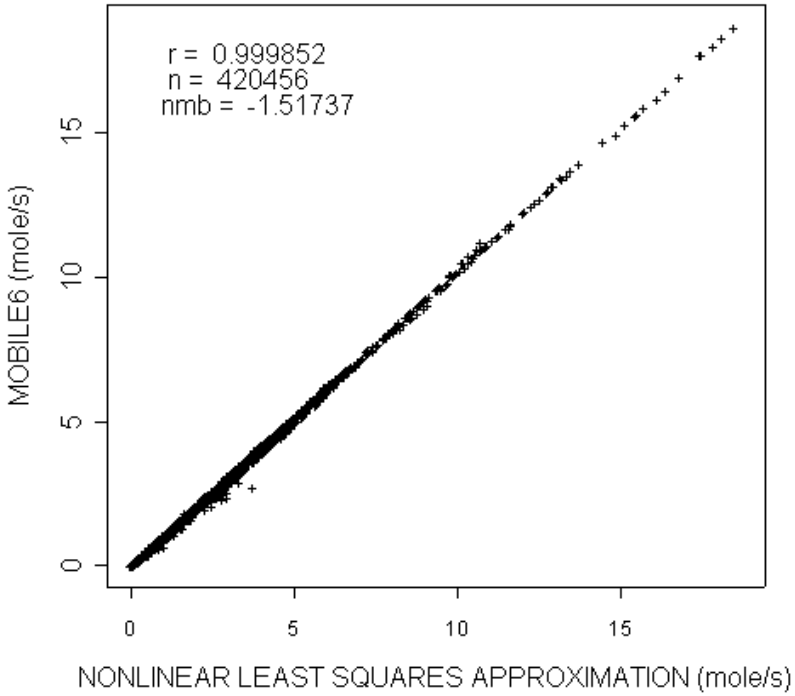
NE Domain Mobile6 vs. Regression: NO_x

July 19, 2004 retrospective

Monday



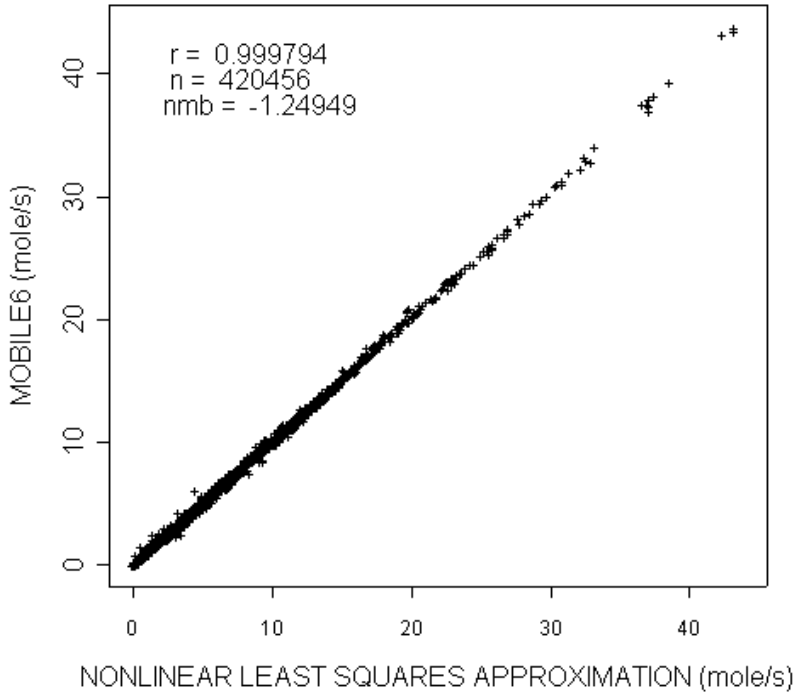
Saturday



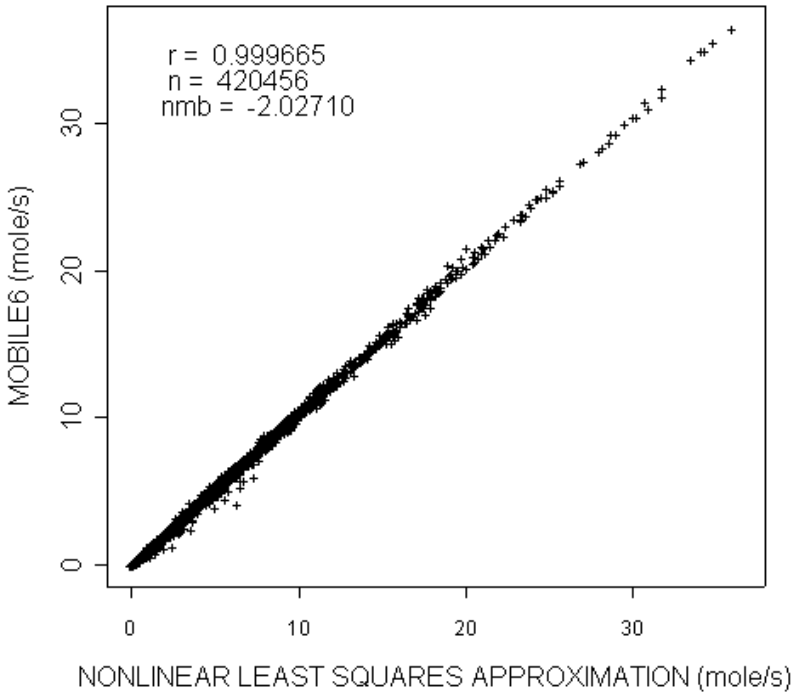
NE Domain Mobile6 vs. Regression: VOC

July 19, 2004 retrospective

Monday



Saturday

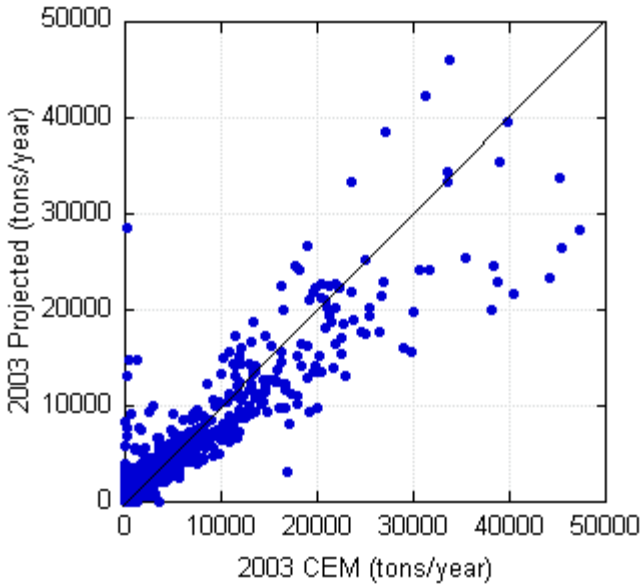


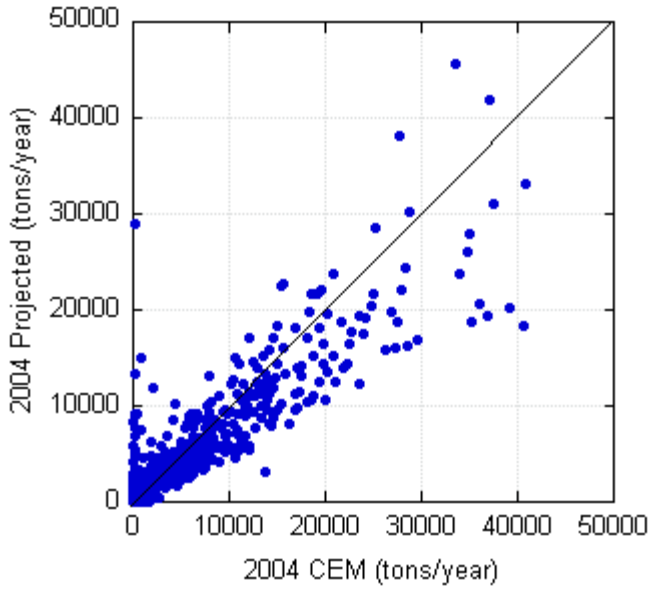
Point Sources

- 2001 NEIv3 inventory (from CAIR); modified EGU NOx emissions using DOE's Annual Energy Outlook (Jan 2004)
- Calculated 2005/2001 NOx annual emission ratios on a regional basis (from DOE data)
- Non-EGU sector: 2001 NEIv3

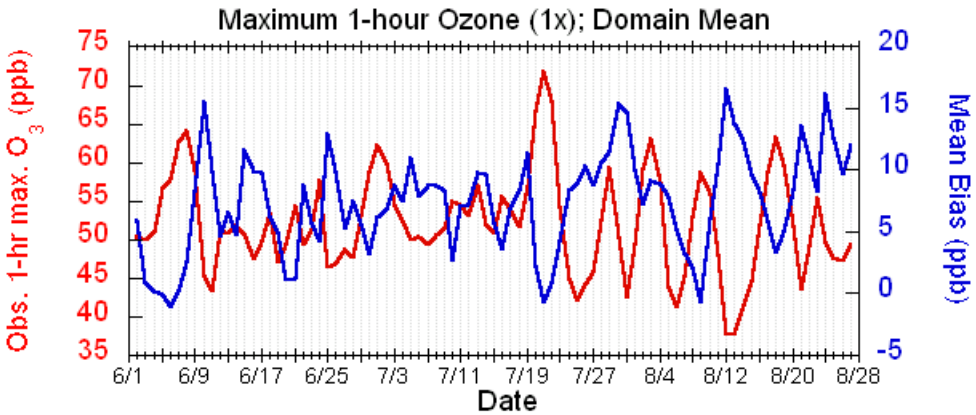
Point Sources: Comparison with CEM Data

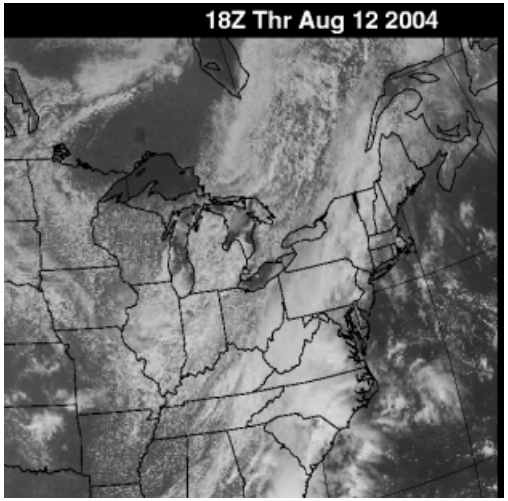
NO_x Emissions

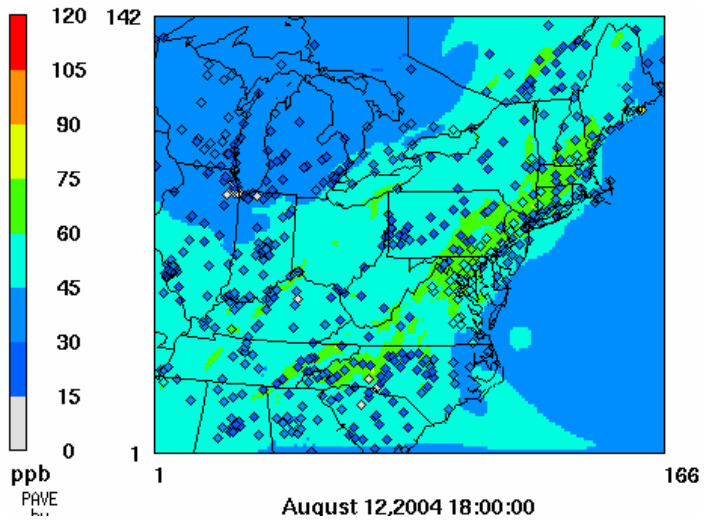




Recap of 2004 AQF Performance







Over predictions at surface (low concentrations) during cloudy conditions diagnosed due to:

- -Unrealistic “top-down” mixing in model’s convective cloud scheme
  - *- Magnified due to over predictions in free troposphere*
- -Attenuation of below cloud photolysis

CMAQ Configuration

- **Advection**
  - Horizontal: *Piecewise Parabolic Method*
  - Vertical: *Upstream with rediagnosed vertical velocity to satisfy mass conservation*
- **Turbulent Mixing**
  - K-theory; PBL height from Eta
  - Minimum value of K_z allowed to vary spatially depending on urban fraction (f_{urban})
    - $K_z = 0.1\ m^2/s$, $f_{urban} = 0$
    - $K_z = 2.0\ m^2/s$, $f_{urban} = 1$
  - allows min. K_z in rural areas to fall off to lower values than urban regions during night-time
  - prevents precursor concentrations (e.g., CO, NOx) in urban areas from becoming too large at night; reduced mixing intensity) in non-urban areas results in increased night-time O3 titration

CMAQ Configuration (contd.)

- **Gas phase chemistry**
  - *CB4 mechanism with EBI solver*
  - Below cloud attenuation based on ratio of radiation reaching the surface to its clear-sky value
    - Closer linkage with Eta
- **Cloud Processes**
  - Mixing and aqueous chemistry
  - Sub-grid scheme based on modifications to RADM formulation; “switch-off” entrainment from above clouds
    - Used in Eastern U.S. (3x) domain
  - Tested a new “in-cloud” mixing based on the Asymmetric Convective Mixing (ACM) model (Pleim and Chang, 1992, *JGR*)
    - Used in Continental U.S. (5x) domain

CMAQ Configuration (contd.)

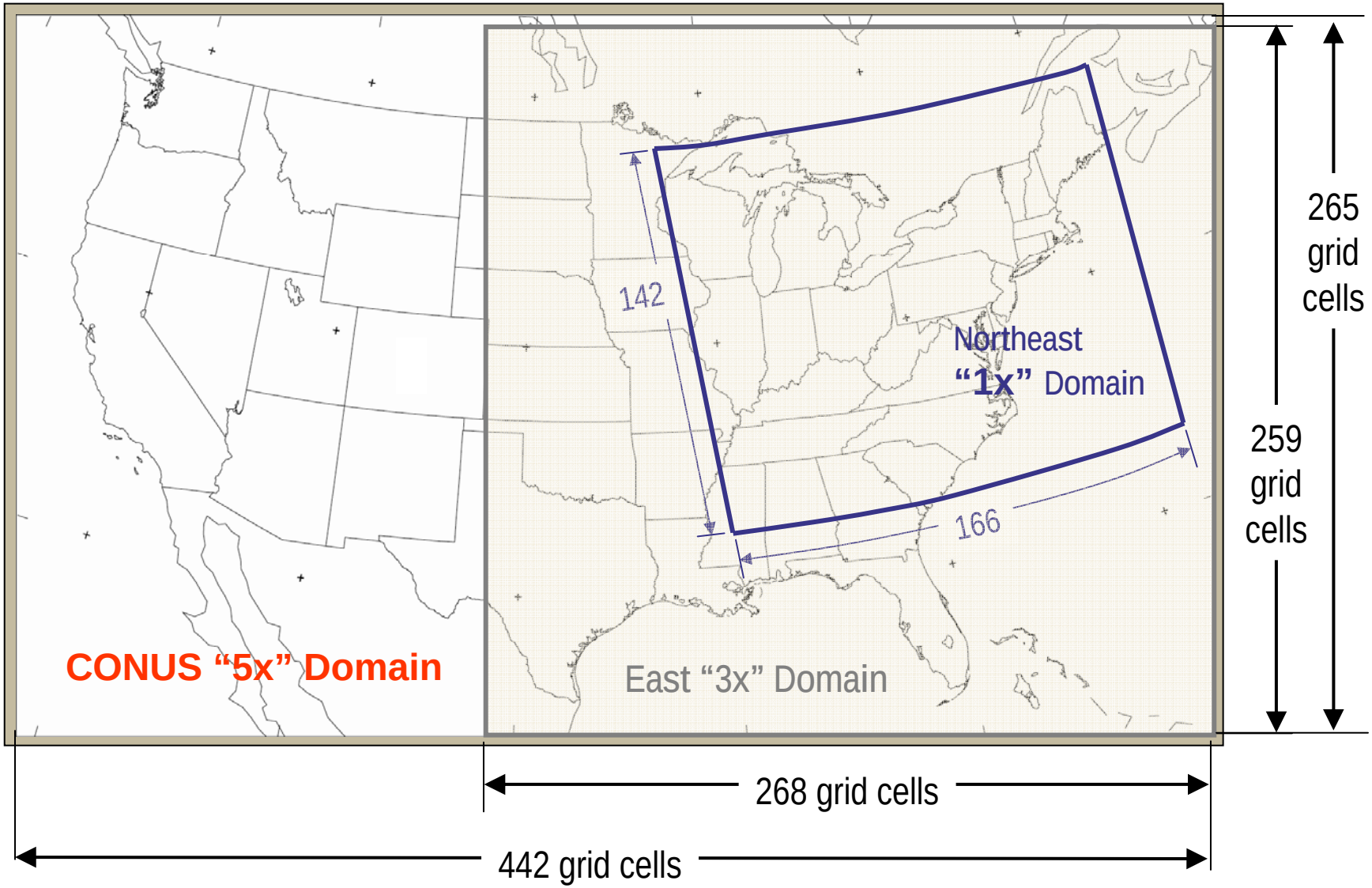
- **Deposition**
  - Dry : M3dry modified to use Eta land surface parameters
  - Wet
- **Aerosols**
  - Lognormal size distribution (σ_g and D_g)
    - Aitken mode (0-0.1 µm)
    - Accumulation mode (0.1-2.5 µm)
    - Coarse (PM10 - PM2.5)
  - *2004 release version*
    - *Binkowski and Roselle, JGR, 2002*

CMAQ Modeling Domains

Experimental PM forecasts on 3x

Ozone forecasts on all three domains

12 km resolution



Lateral Boundary Condition Specification

- A key uncertainty in long term modeling over limited area domains
  - *Determines "model background"*

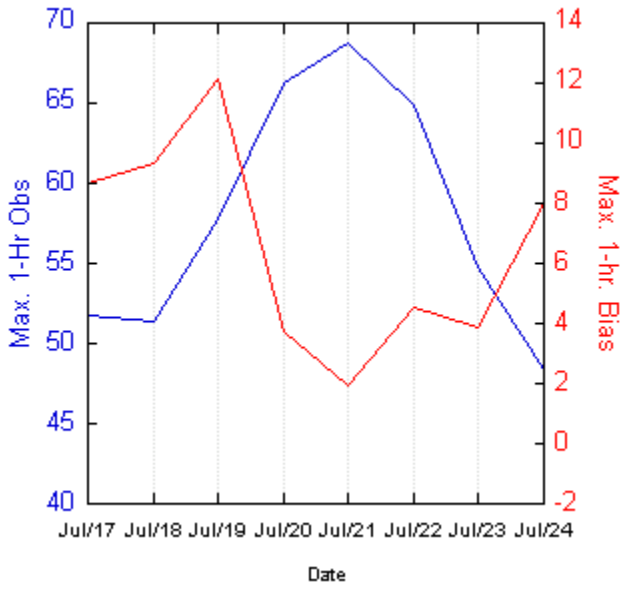
- **Approach**: Combination of
  - Surface to 6km: static default profiles
    - "Clean" tropospheric background values
  - Above 6km: O_3 profiles from NCEP's Global Forecast System (GFS) model
    - O_3 is a 3-d prognostic variable
    - Initialized with Solar Backscatter Ultra-Violet (SBUV-2) satellite observations
  - Changes implemented during season
    - 5x: Restricted to top most CMAQ layer; then discontinued use
    - 3x: Restricted to top most CMAQ layer

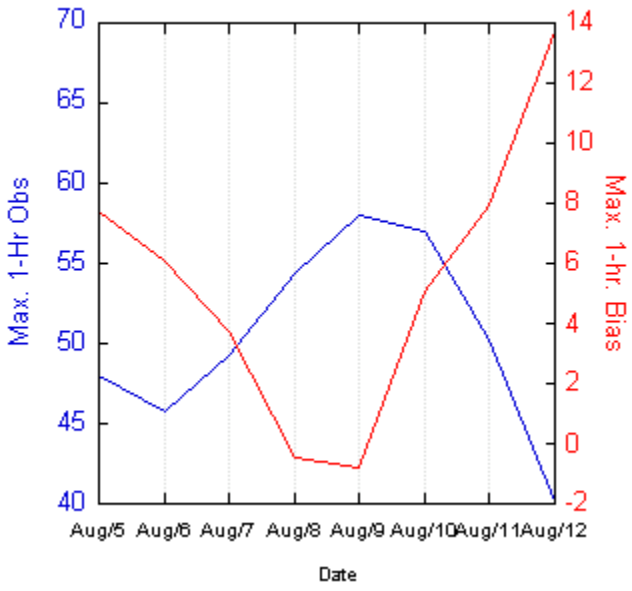
Retrospective Sensitivity Simulations
Organization of Simulations

- **2004 Base**: 2004 Operational run
- **S0**: Reflects impacts due to upgrades to Eta
- **S1**: S0 + photolysis attenuation based on Eta radiation fields
- **S2**: S0 + ACM-type cloud mixing
- **S3**: S0 + Entrainment from above clouds turned-off
- **S4**: S1+S2 (ACM + Photolysis change)
- **S5**: S1+S3 (above cloud entrainment off + Photolysis change)

Retrospective Sensitivity Simulations
Analysis Time Periods

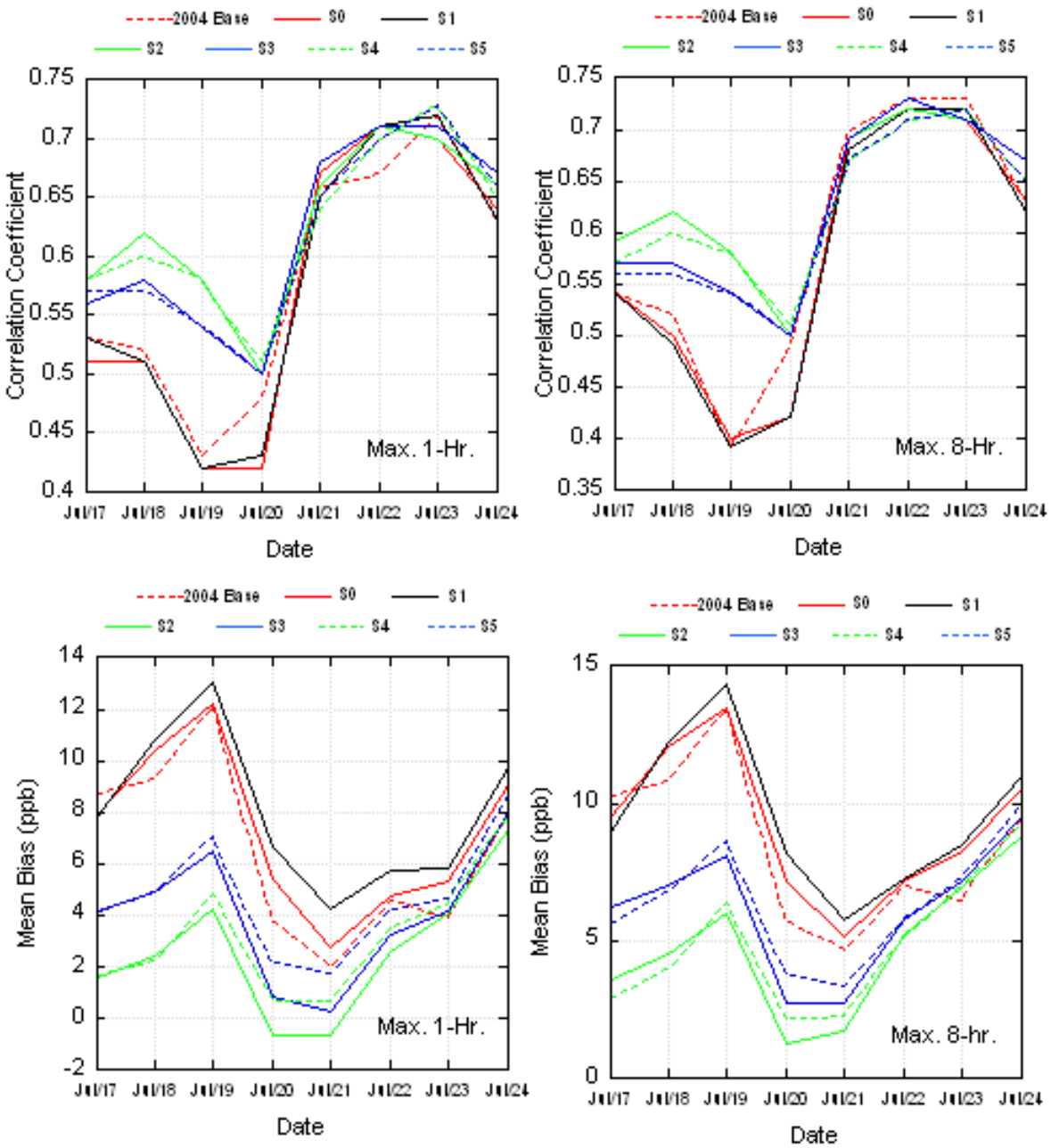
- **Time Periods**
  - 12Z July 16, 2004 – 12Z July 25, 2004
  - 12Z August 4, 2004 – 12Z August 13, 2004





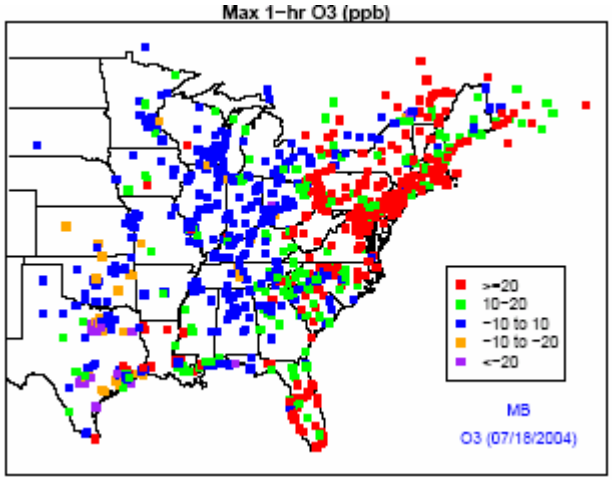
Results from 2004 air quality forecasts

Retrospective Sensitivity Performance Summary: July 2004 Case

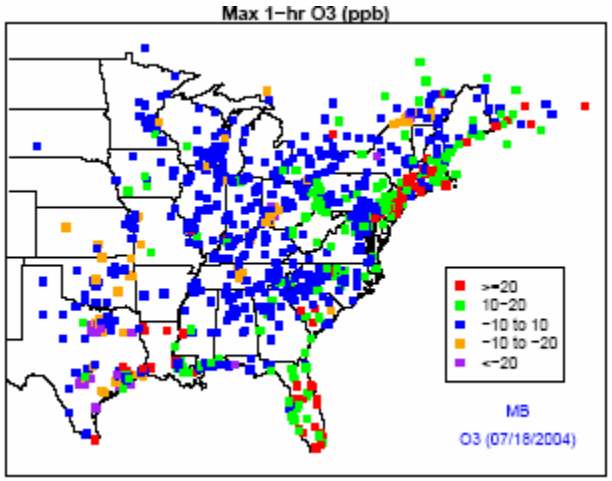


Max 1-hr O_3 Mean Bias Spatial Distribution: July 19, 2004

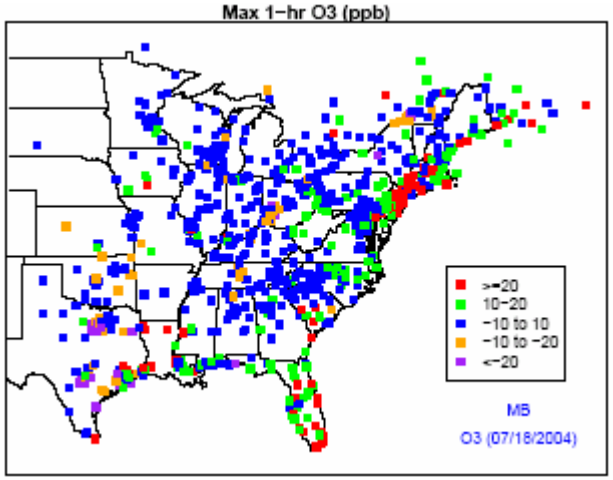
S0



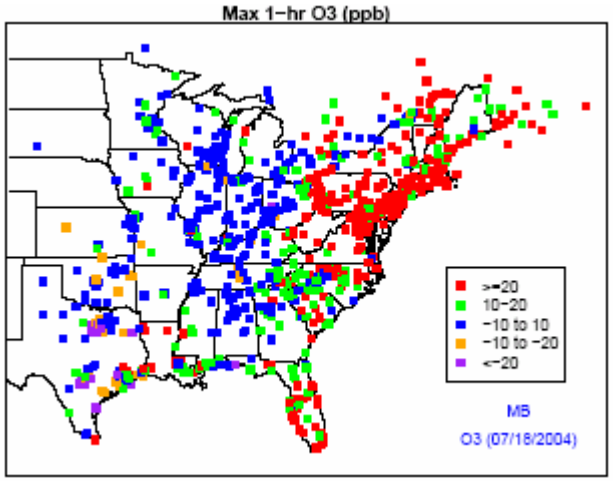
S2



S4



S1



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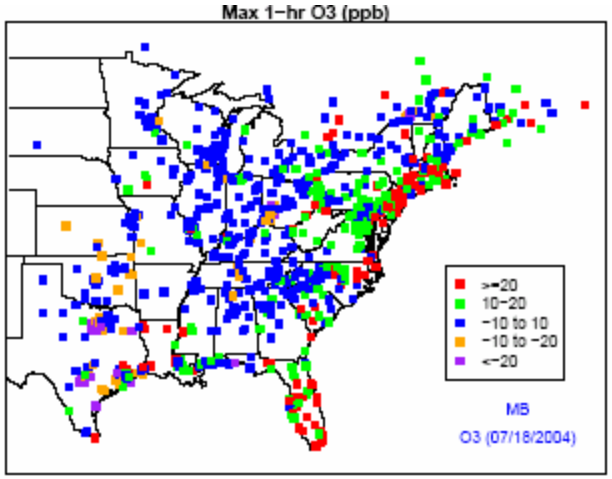
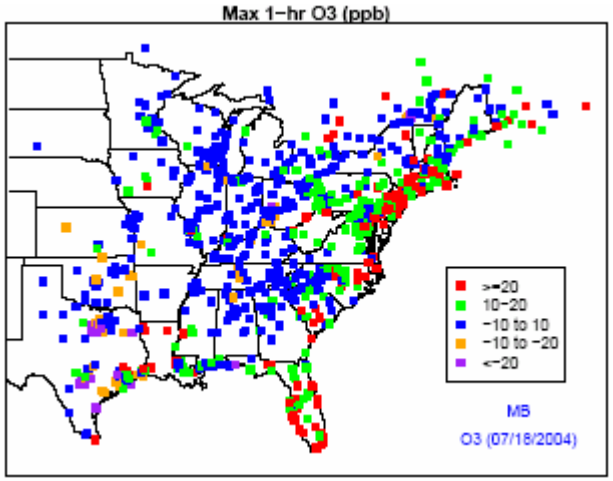
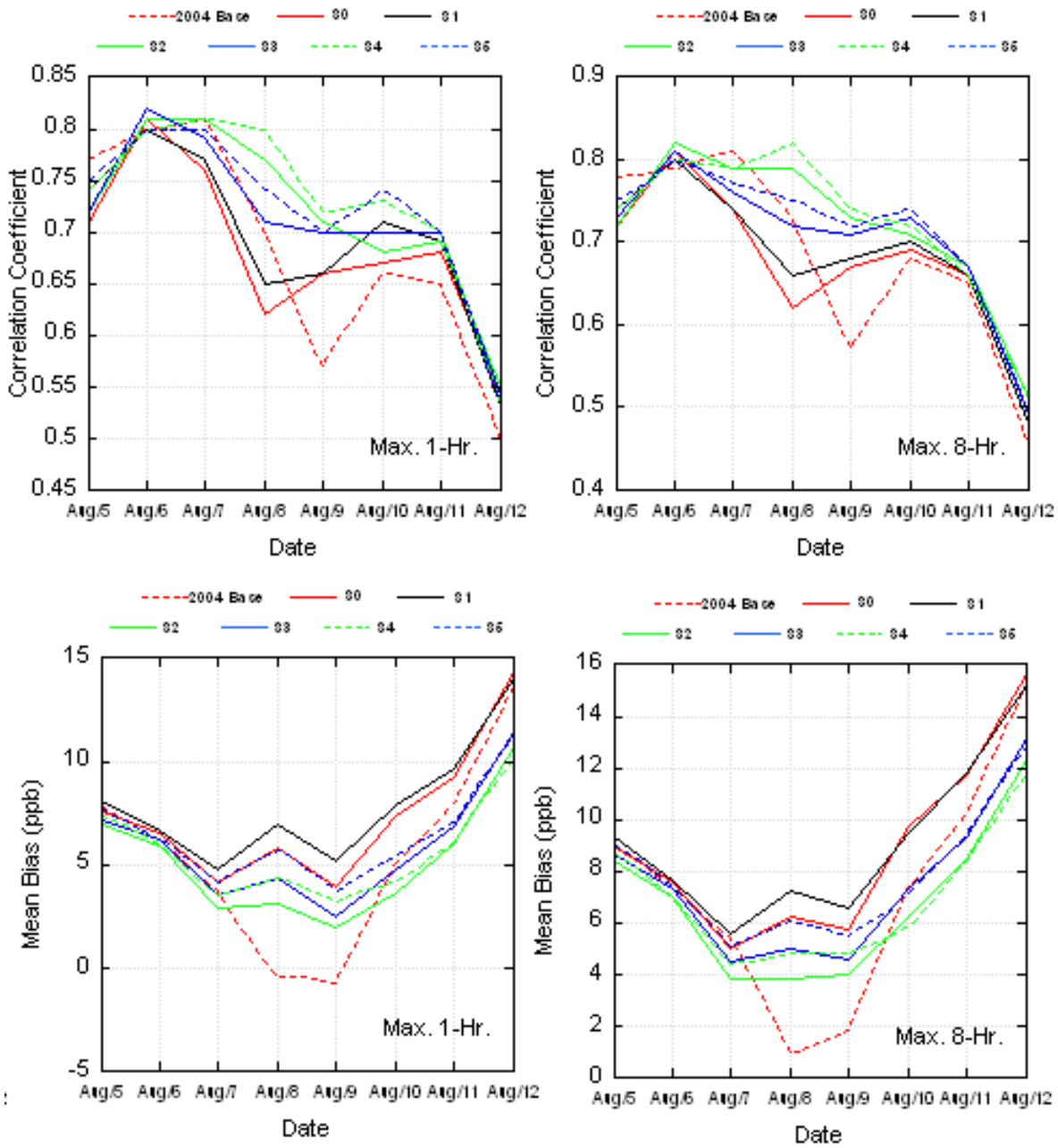


S5

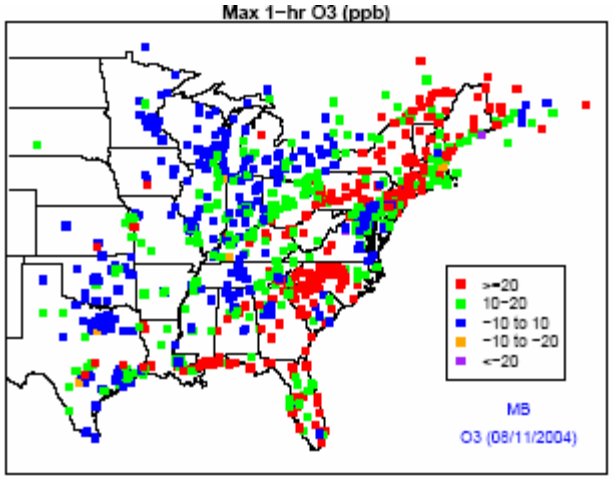


Retrospective Sensitivity Performance Summary: August 2004 Case

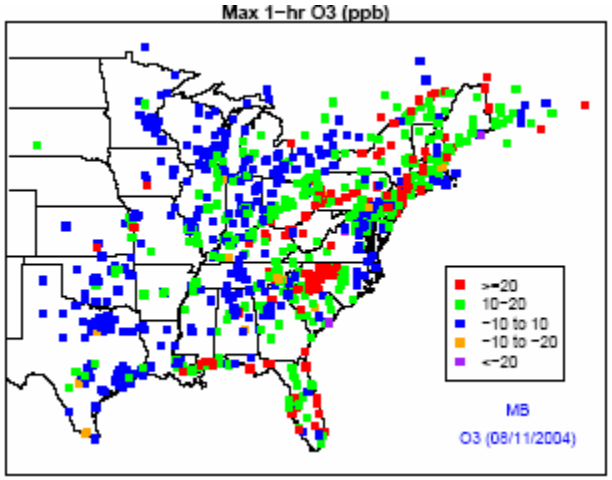


Max 1-hr O_3 Mean Bias Spatial Distribution: August 12, 2004

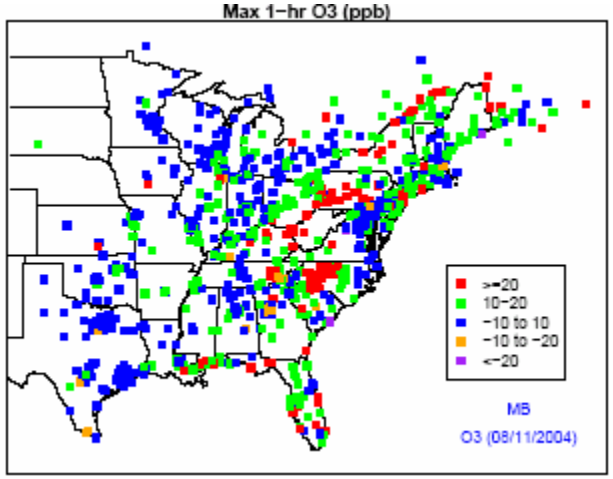
S0



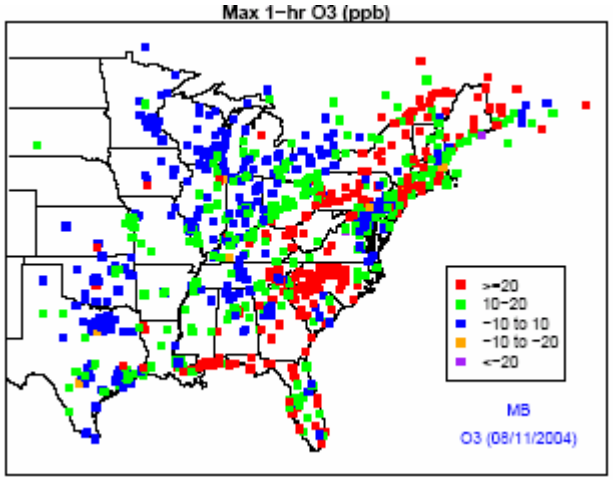
S2



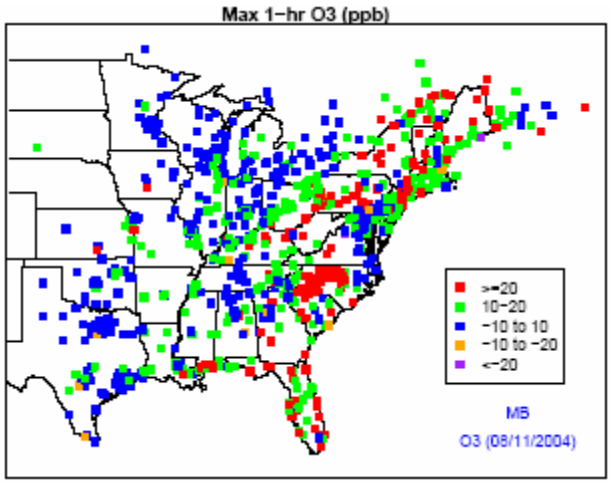
S4



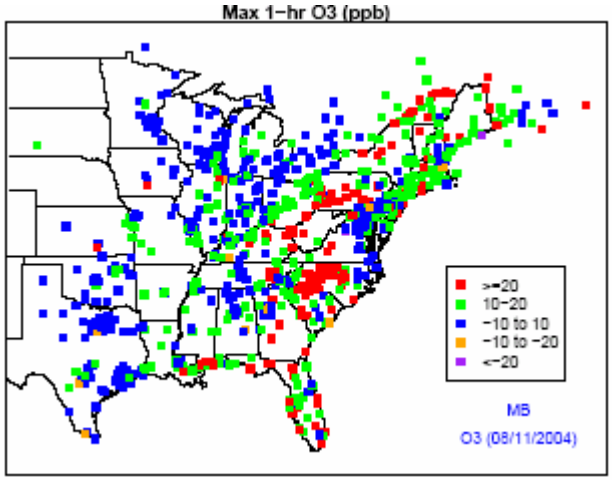
S1



S3

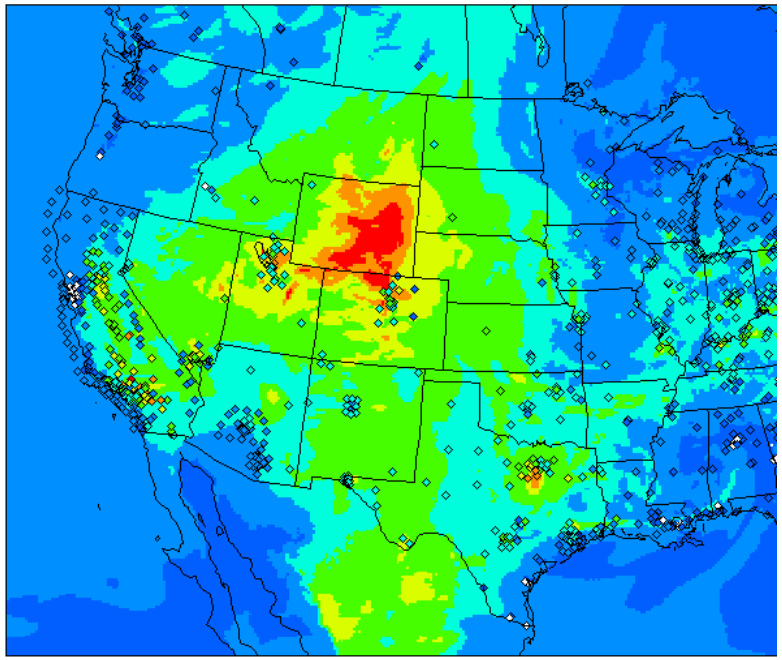


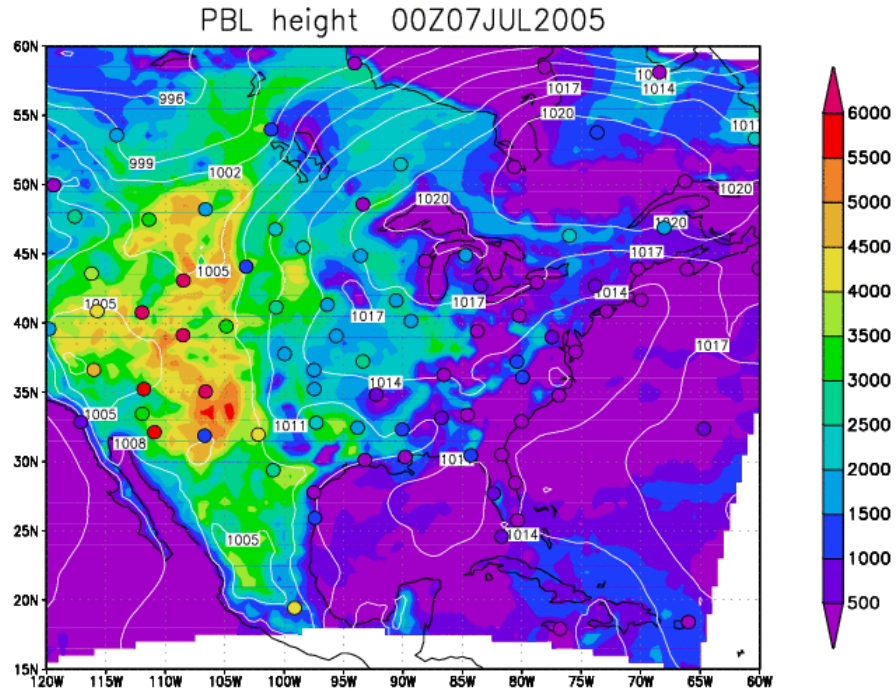
S5



Motivation for change in use of GFS LBCs

Example: July 7, 2005 00Z





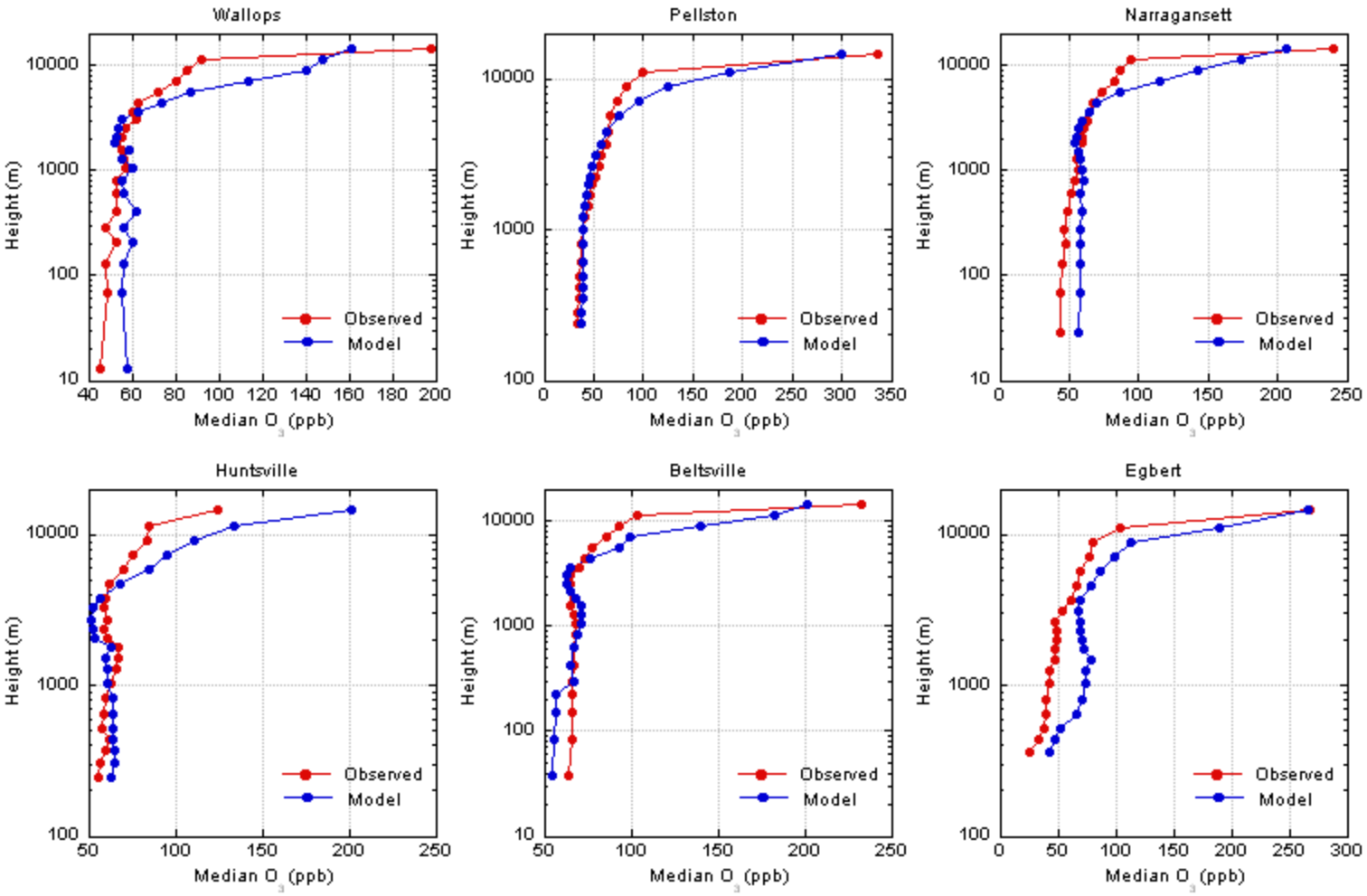
Courtesy: M. Tsidulko

Downward mixing of high O_3 aloft through deep PBL in the west

➡ How good is the representation of model's FT O_3 values?

O_3 Model Performance: Aloft

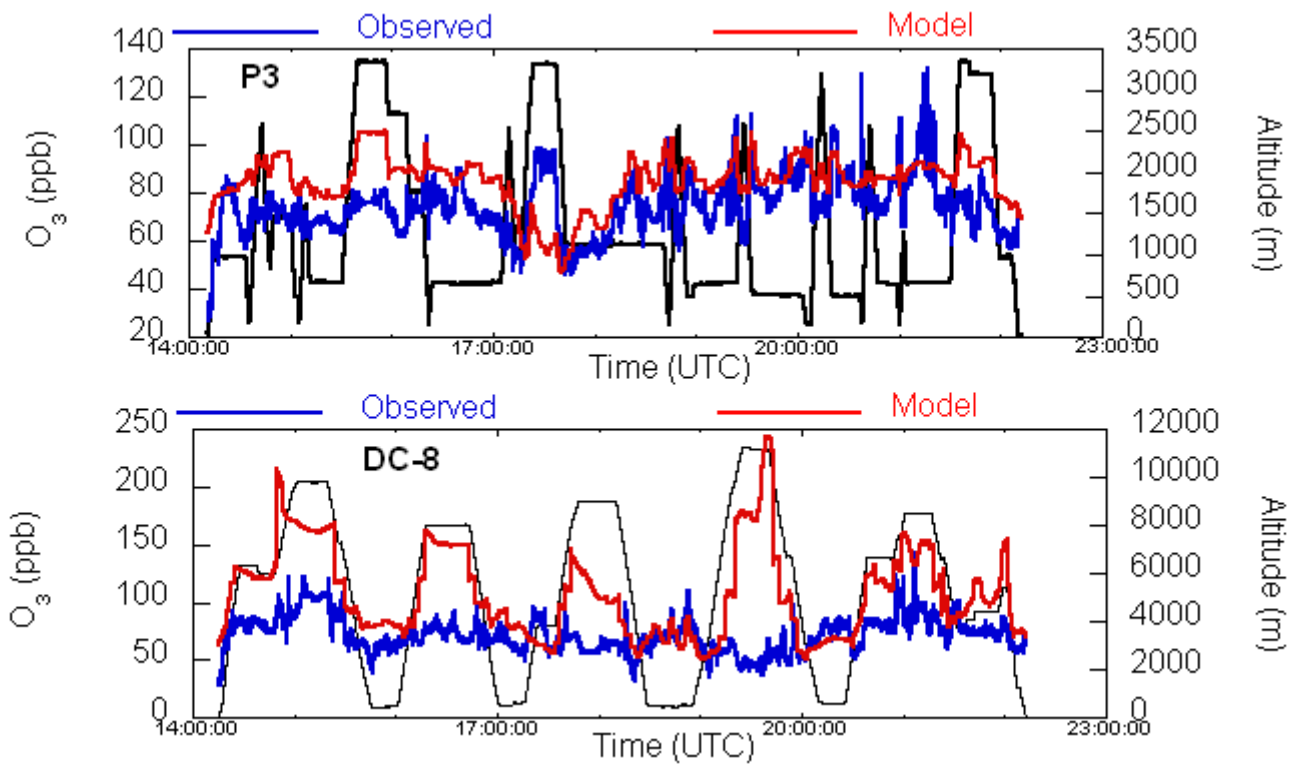
July-August 2004 Median Profiles against IONS Ozonesonde Data



Over predictions above 6 km: Impact from GFS derived LBC and coarse model resolution in FT

O_3 Model Performance: Aloft

P3 and DC8 Flights on July 20, 2004



Over predictions at surface during cloudy conditions diagnosed due to:

- -Unrealistic “top-down” mixing in model’s convective cloud scheme
  - *- Magnified due to FT over predictions*
- -Attenuation of below cloud photolysis

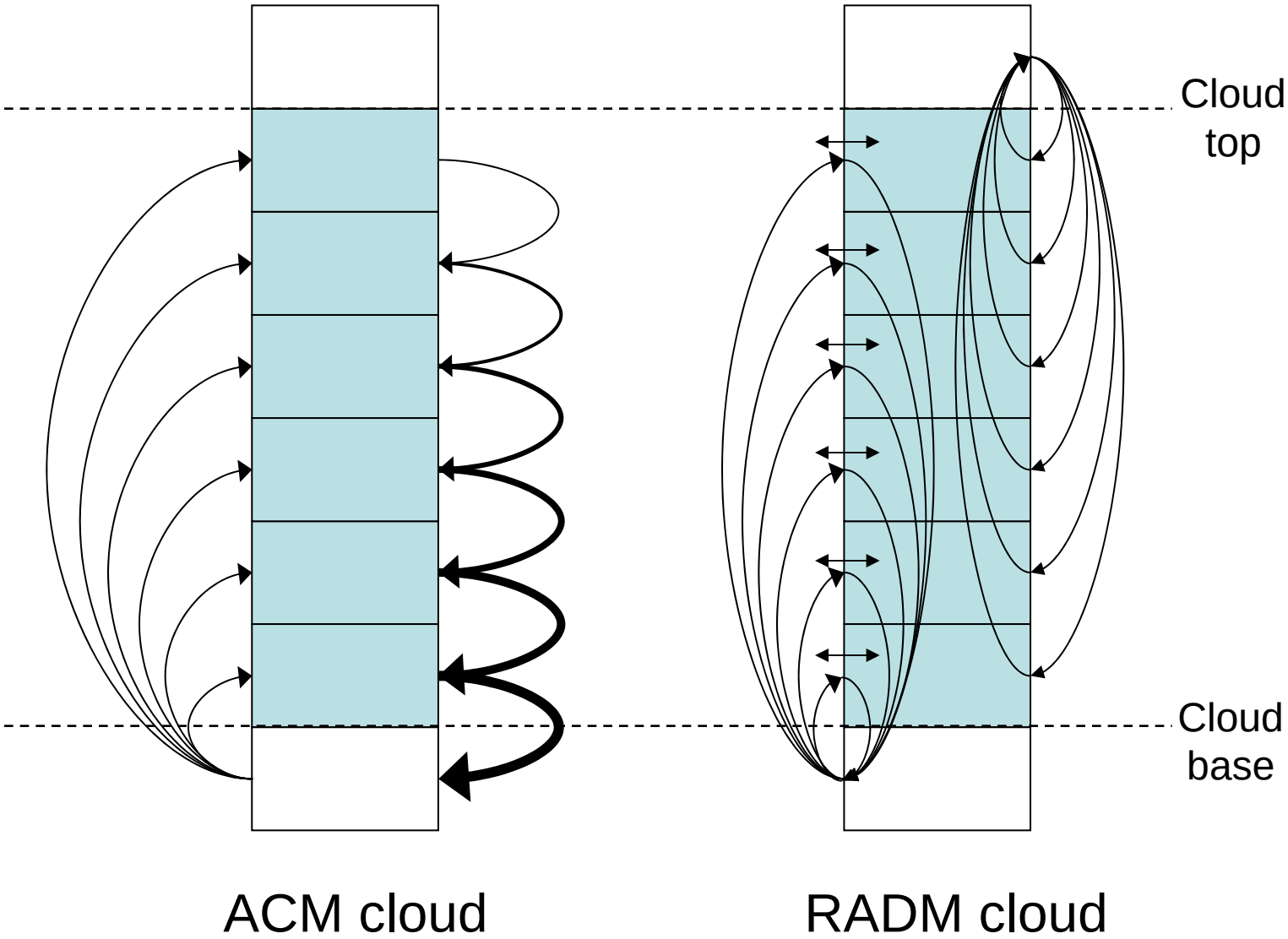
Summary

- Over-predictions in free tropospheric O_3 can be attributed to GFS derived LBCs combined with coarse vertical model resolution
  - Resulted in surface over-predictions in regions with complex terrain and deep PBL
- Surface level over-predictions at low O_3 range related to representation of cloud processes
  - Top-down mixing
  - Photolysis attenuation
- Enhancements to the sub-grid cloud scheme in CMAQ resulted in improvements in performance for surface O_3 forecast
  - Implemented changes are a first step
  - Scope for further improvement

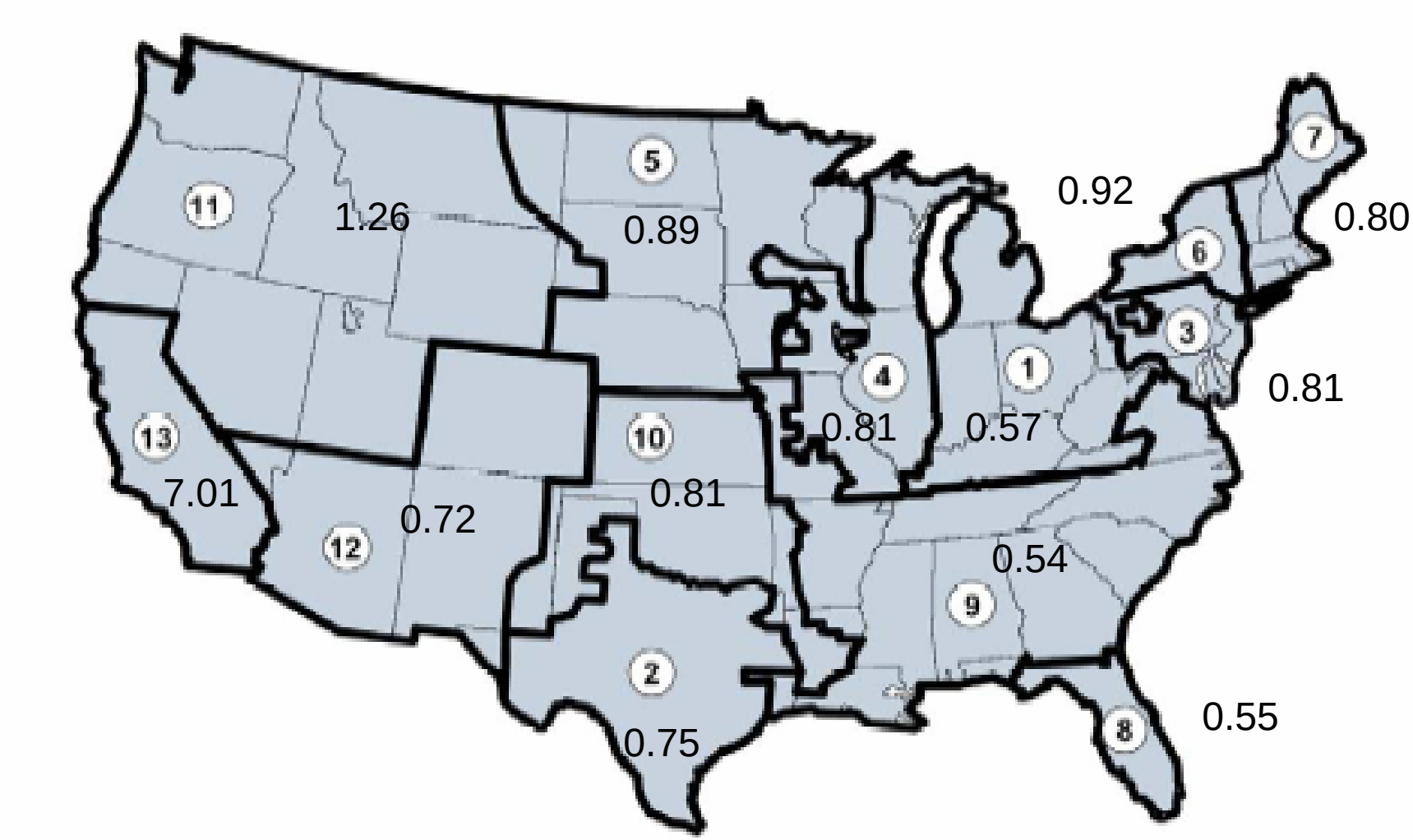
Disclaimer: *The research presented here was performed under the Memorandum of Understanding between the U.S. Environmental Protection Agency (EPA) and the U.S. Department of Commerce's National Oceanic and Atmospheric Administration (NOAA) and under agreement number DW13921548. This work constitutes a contribution to the NOAA Air Quality Program. Although it has been reviewed by EPA and NOAA and approved for publication, it does not necessarily reflect their views or policies.*

Supplemental Slides

Cloud Mixing: Conceptual View



EGU NO_x adjustments 2005/2001 by region for Point Source Inventory



Source: Department of Energy Annual Energy Outlook
http://www.eia.doe.gov/oiaf/aeo/index.html