United States Environmental Protection Agency

The Community Multiscale Air Quality (CMAQ) Model:

Model Configuration, Enhancements, and Testing for 2008 Air Quality Forecasting

SCIENCE

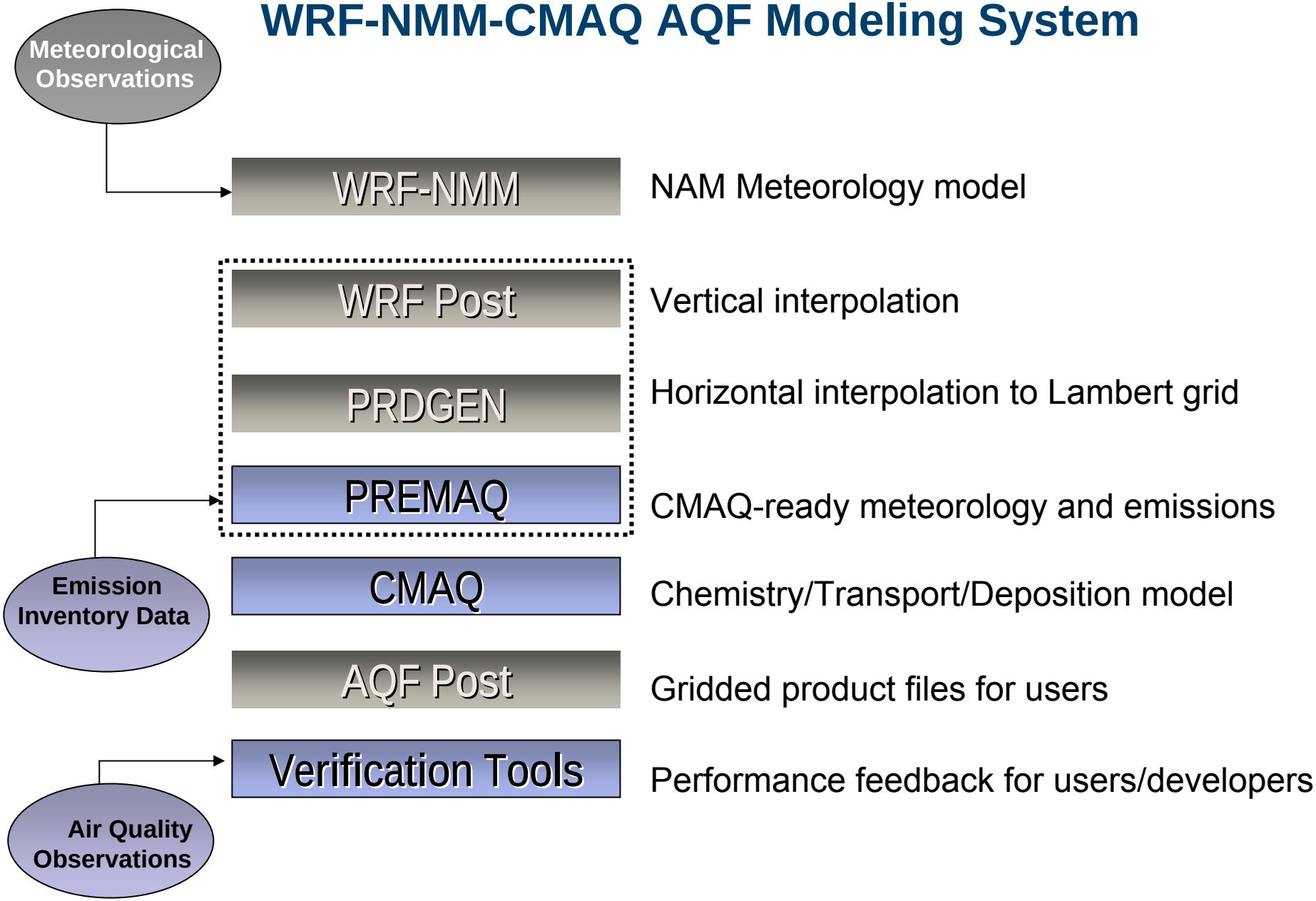
Technical Workshop on Air Quality Predictions
September 16, 2008

Atmospheric Modeling Division
National Exposure Research Laboratory

Contributors:

- **AMD**
  - AnnMarie Carlton
  - Brian Eder
  - Jerry Herwehe
  - Rohit Mathur
  - Tanya Otte
  - Jon Pleim
  - George Pouliot
  - S.T. Rao
  - Kenneth Schere
  - David Wong
  - Jeff Young
- **STC**
  - Tianfeng Chai
  - Daiwen Kang
  - Hsin-Mu Lin
  - Daniel Tong
  - Shaocai Yu
- **NWS**
  - Paula Davidson
  - Jeff McQueen
  - Pius Lee
  - Marina Tsidulko
  - Youhua Tang

WRF-NMM-CMAQ AQF Modeling System



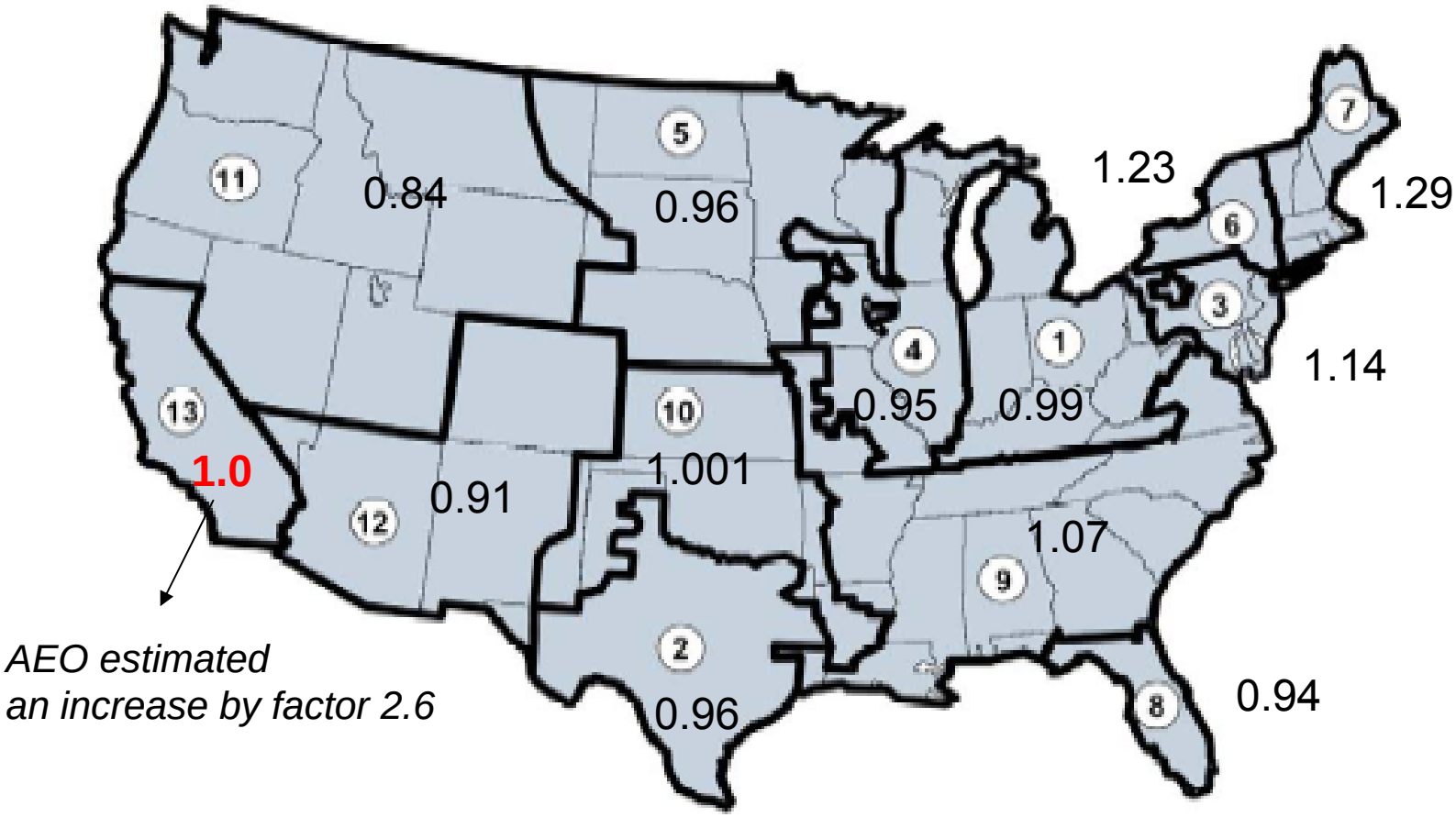
CMAQ Configuration

- **Advection**
  - **Horizontal**: *Piecewise Parabolic Method*
  - **Vertical**: *Upstream with re-diagnosed vertical velocity to satisfy mass conservation*
- **Turbulent Mixing**
  - Asymmetric Convective Model (ACM2); *more later by Jon Pleim*
- **Cloud Processes**
  - Mixing and aqueous chemistry
  - Scavenging and wet deposition
  - "In-cloud" mixing based on the Asymmetric Convective Mixing
- **Dry Deposition**
  - M3dry modified to use NAM land surface parameters
  - *Estimated V_d sensitive to NAM LSM changes*
- **Gas-Phase Chemistry**
  - ODE Solver: EBI solver
  - CBM-IV in Operational model
  - CB05 in experimental/developmental model
  - *Below cloud attenuation based on ratio of NAM radiation reaching the surface to its clear-sky value*
- **Aerosols**
  - Superposition of 3 log-normal modes (aitken, accumulation, coarse)
  - SO_4^{2-}, NO_3^-, NH_4^+, OC, EC, Na+, Cl^-, other primary
  - Chemically inactive coarse mode in current version

Emission Updates for 2008

- **Area and Non-road sources**
  - 2005 NEI v1
  - Non-road emissions based on estimates from EPA Office of Transportation and Air Quality (OTAQ)
  - Wild/Prescribed fires: 1996-2002 average
- **Emissions for Canada**
  - 2000 Base year estimates
- **Emissions for Mexico**
  - BRAVO 1999 inventory for point and area
  - Included surrogates for spatial allocation of area sources
- **Biogenic Sources**
  - Biogenic Emissions Inventory System (BEIS) v3.13
- **Mobile Sources**
  - In previous years used T-based linear regression approximation to MOBILE-6
    - VMT projections were available till 2007
    - Impact of T-variations is small ~2%
    - 2005 OTAQ estimates are 12-15% lower than 2007 AQF estimates
  - Based on-road emissions on 2005 OTAQ estimates to account for recent changes in this sector
- **Point Sources**
  - NO_x and SO_2 using 2006 CEM in conjunction with DOE/AEO projections
  - Other pollutants and non-EGUs: 2005 NEIv1

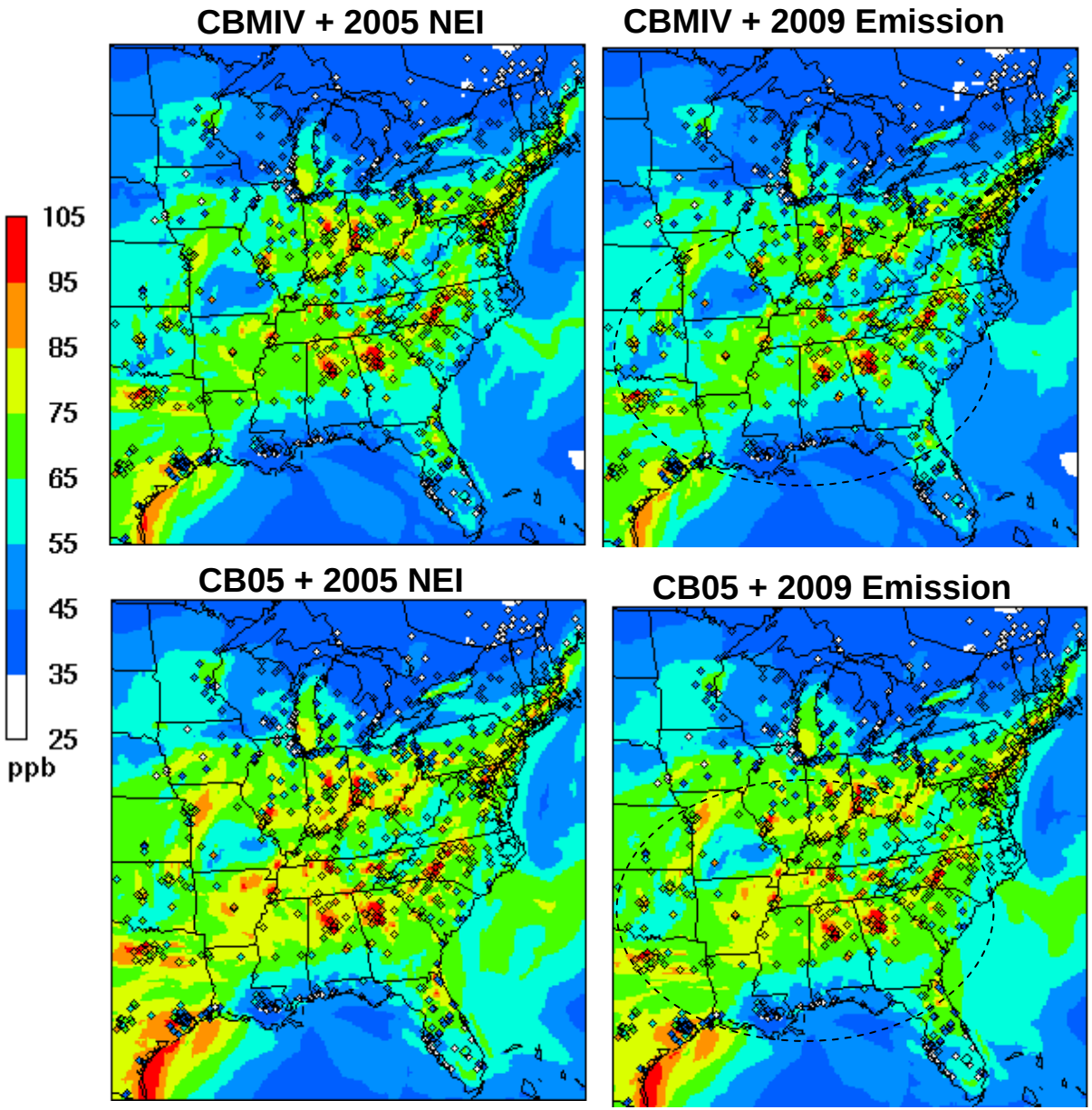
EGU NO_X adjustments 2008/2006 by region



Source: derived from Department of Energy Annual Energy Outlook 2007
http://www.eia.doe.gov/oiaf/aeo/index.html

Mechanism (CBMIV, CB05) and Emission (2005 NEI, 2009) Sensitivity

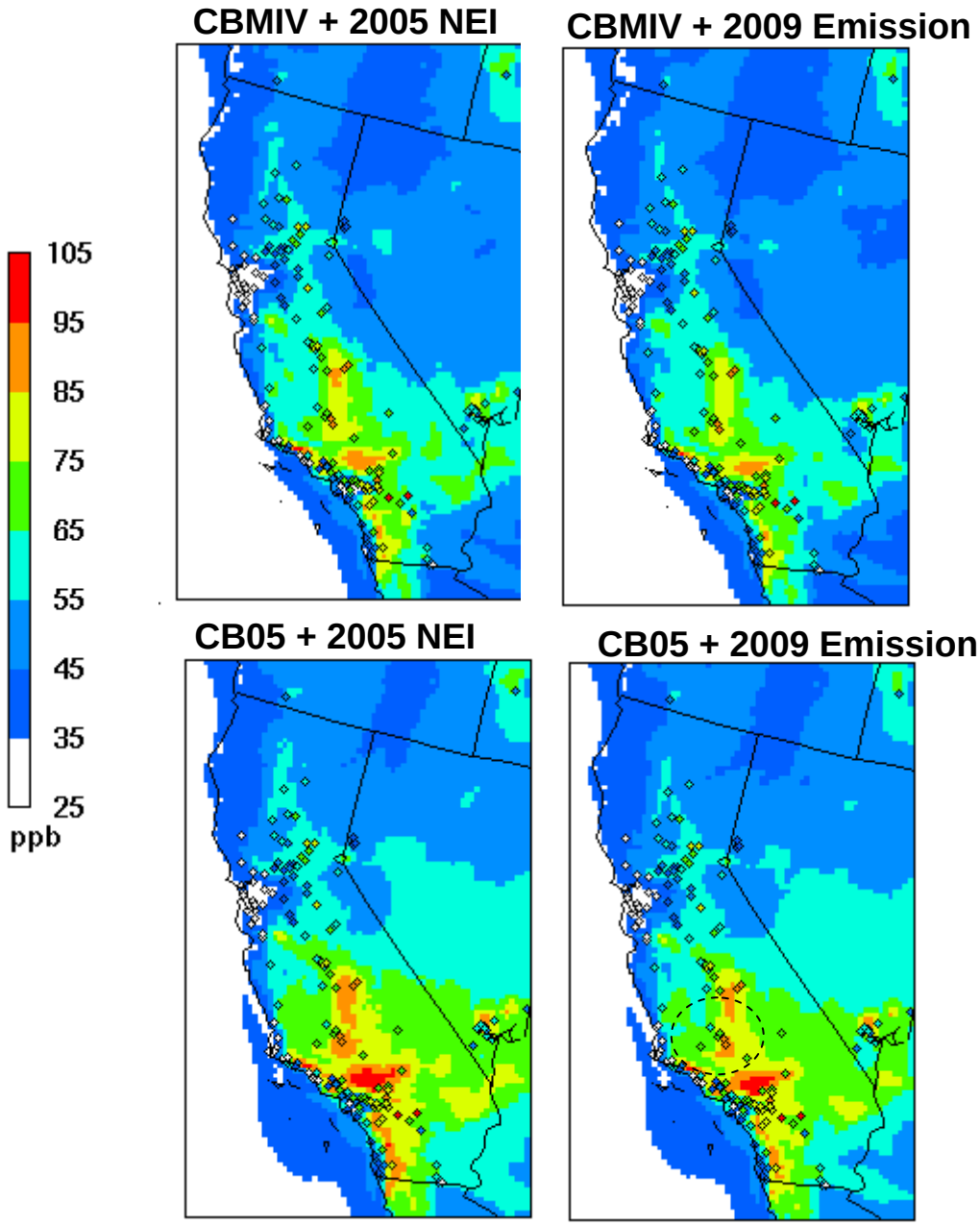
Max. 8-hr O_3: August 15, 2007



- CBM05 generally higher
- CBMIV w/2009 emission estimates may have resulted in low bias in operational run

Mechanism and Emission Sensitivity

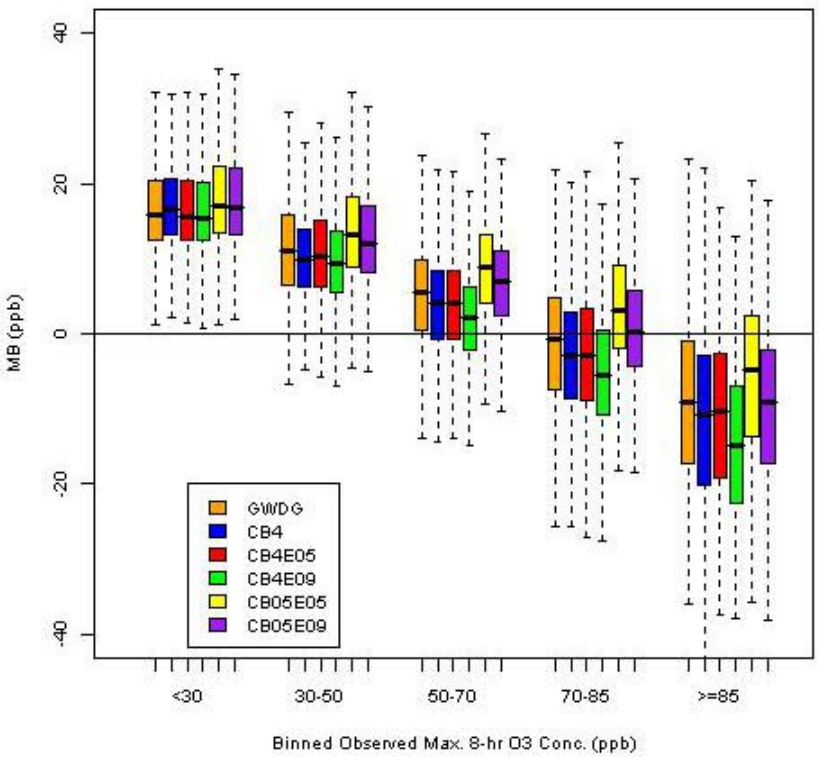
Max. 8-hr O_3: August 15, 2007

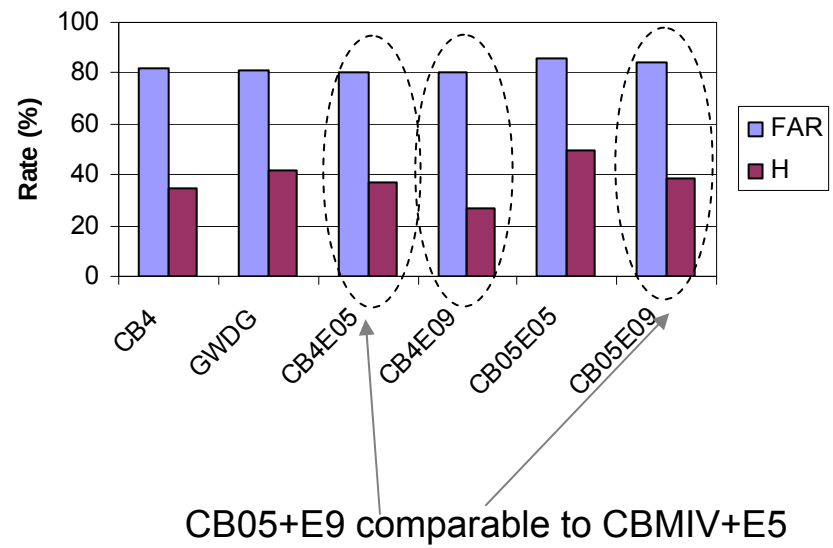


- CBM05 generally higher
- CBMIV w/2009 emission estimates may have resulted in low bias in operational run

Mechanism and Emission Sensitivity

Max. 8-hr O3: August 5-18, 2007



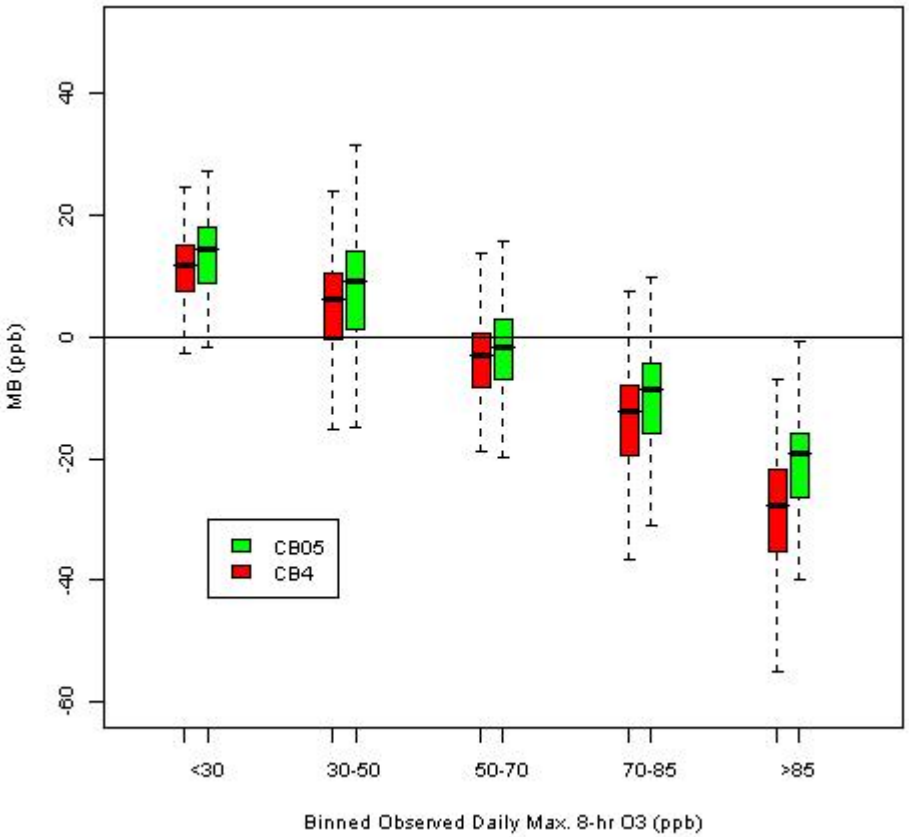


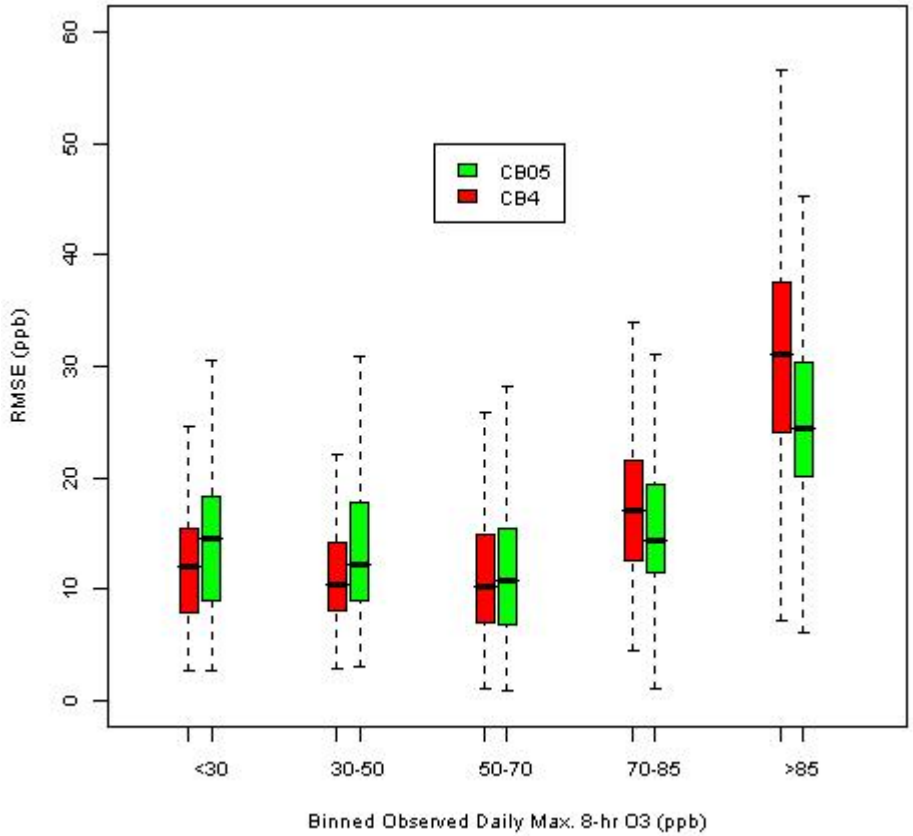
- CB05 exhibits higher bias/error at the low-moderate O_3 mixing ratio range, but lower bias/error for O_3 > 70ppb
- CBMIV with 2009 emission estimates may have deteriorated peak prediction performance for operational model

Mechanism performance assessments should also consider emission uncertainty

CBMIV (Operational) vs. CB05 (experimental) performance

Max 8-hr O_3, CONUS, June 15-Aug. 31, 2008



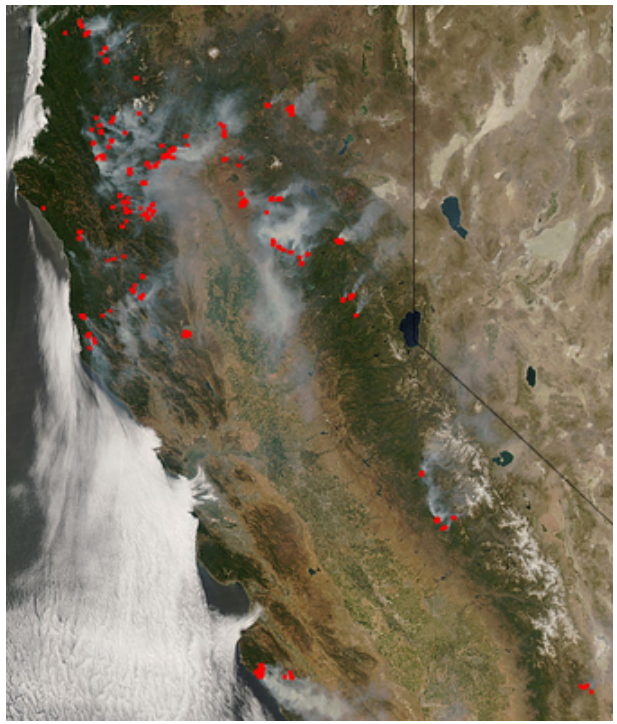


- Lower bias and error with CB05 at moderate-high O_3 mixing ratios
- Higher error in regional statistics due to over-prediction at low mixing ratio range
  - *Could it be for reasons other than chemical mechanism?*

Wildfire Emissions:

Source Characterization and Air Quality Impacts

HMS Fire Detects

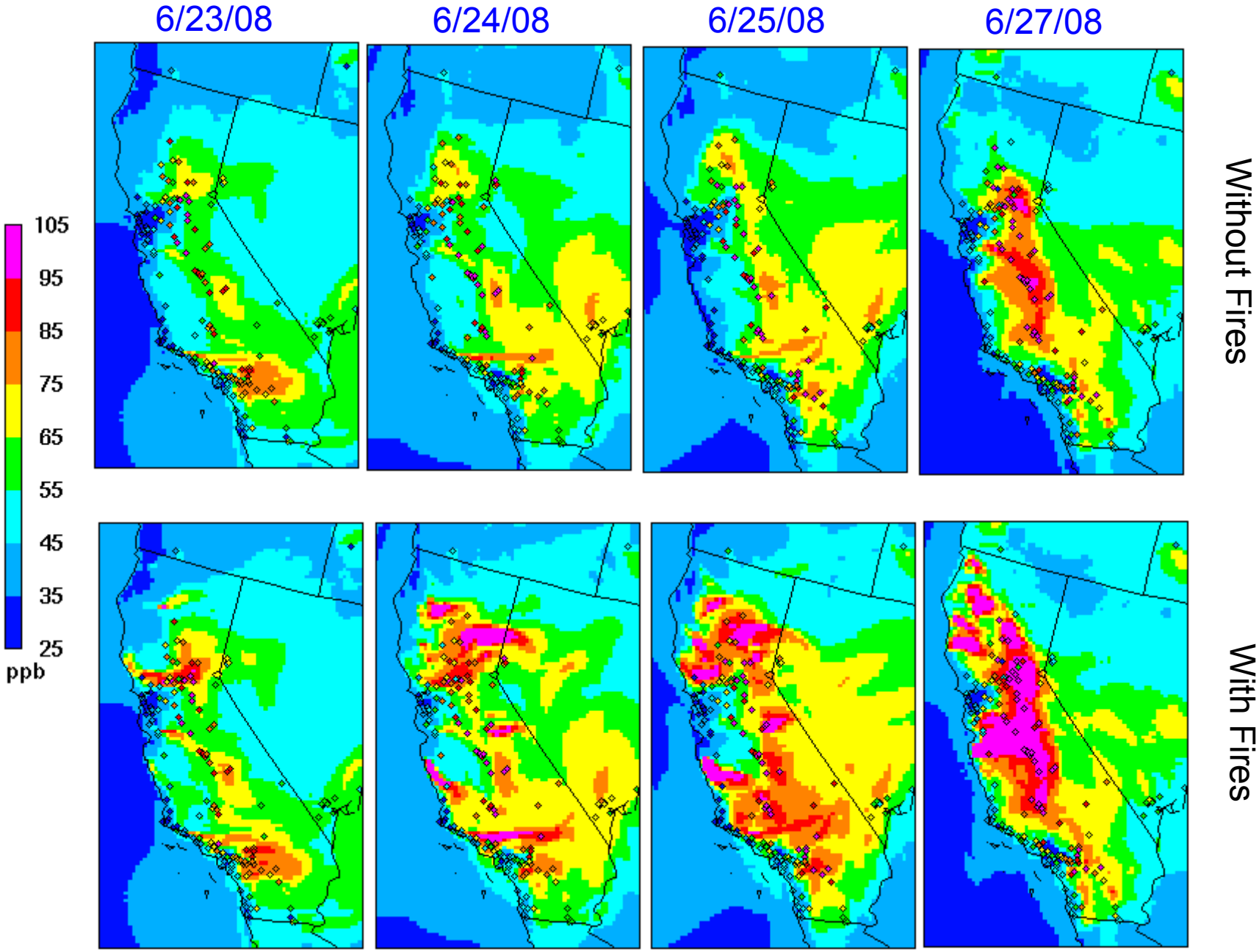


Emissions = (*Fuel Loading*) x (*Acres Burned*) x (*Emission Factor*)

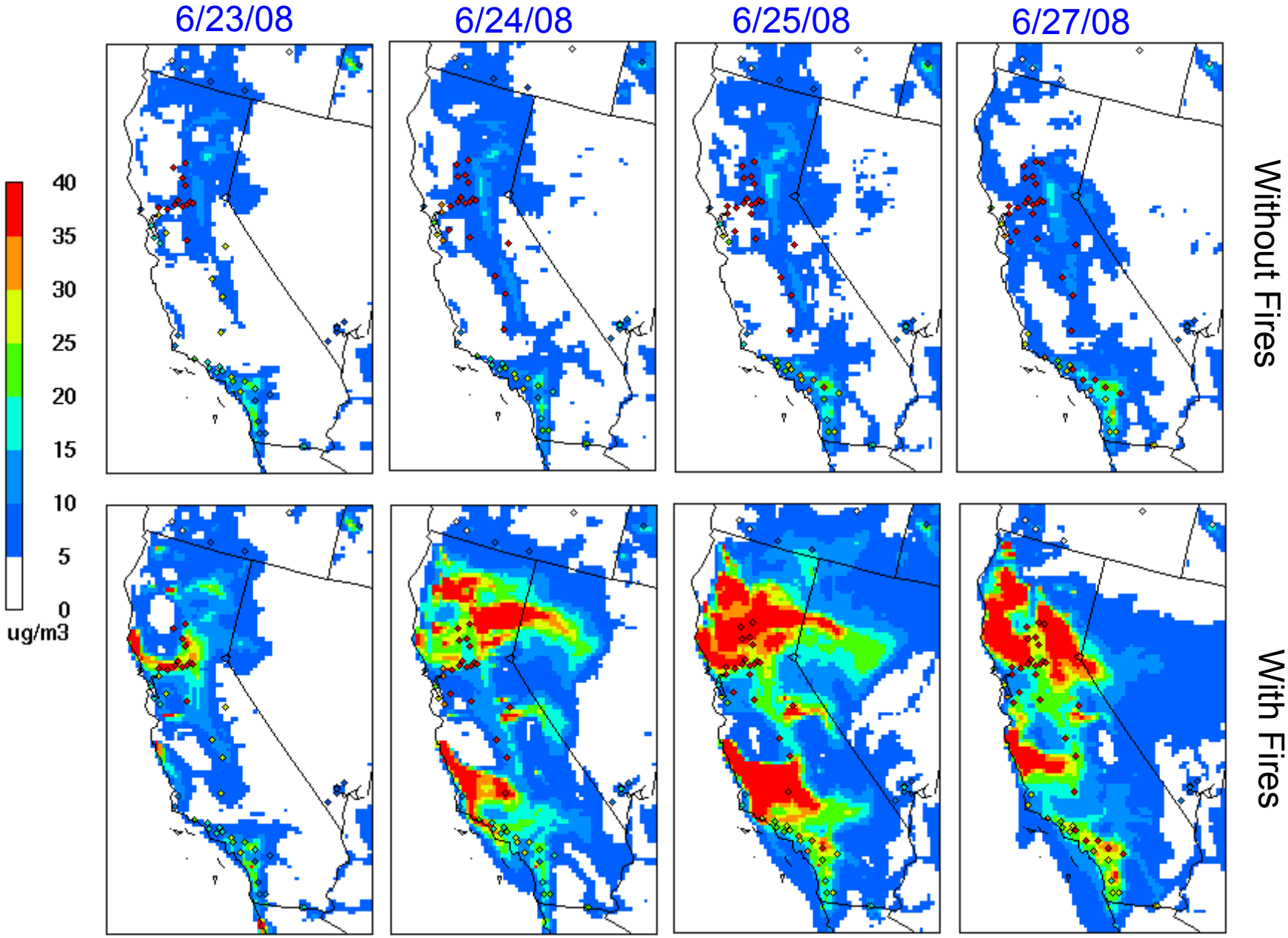
NAM-CMAQ

In subsequent runs:
- Fuel loading based on the National Fire Danger Rating (NFDR) system
- Emission Factors: Fire Emission Production Simulator (FEPS)
  Function of fuel class

Impacts of Wildfire Emissions on Max. 8-hr O_3



Impacts of Wildfire Emissions on Daily-avg. $PM_{2.5}$

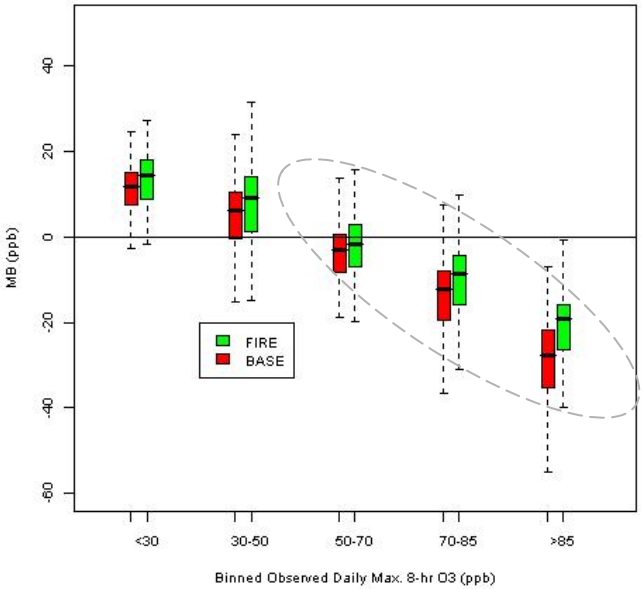


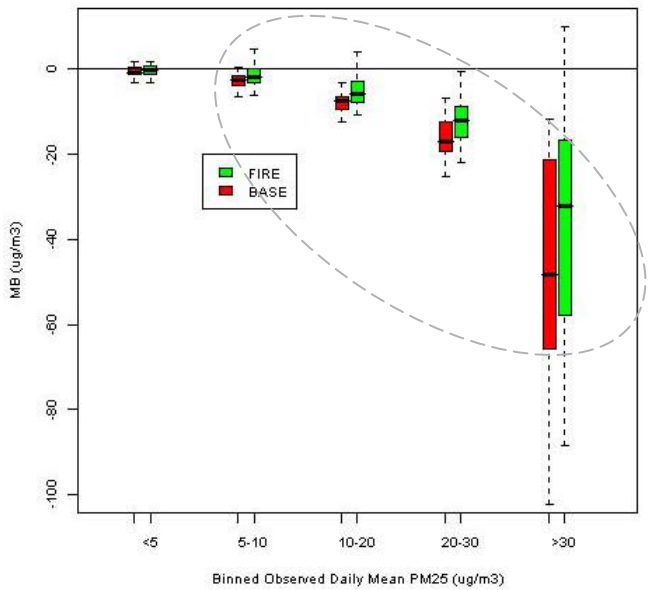
Impact of wildfire emission inclusion on performance for O_3 and $PM_{2.5}$

O_3

$PM_{2.5}$

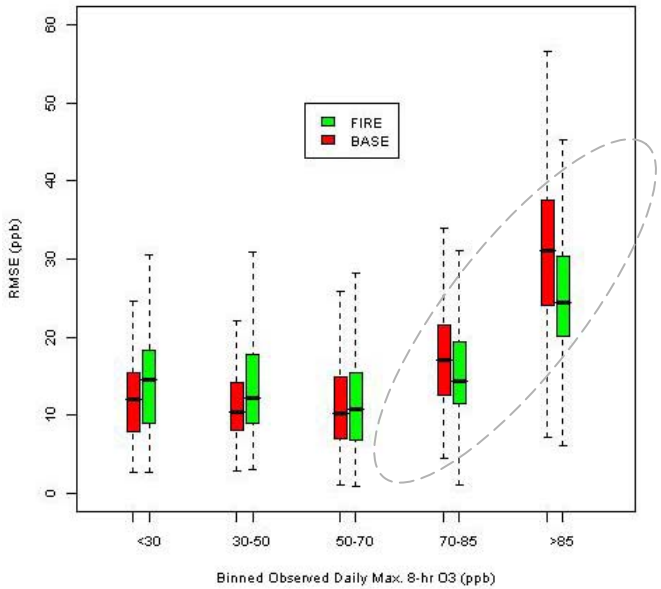
Mean Bias

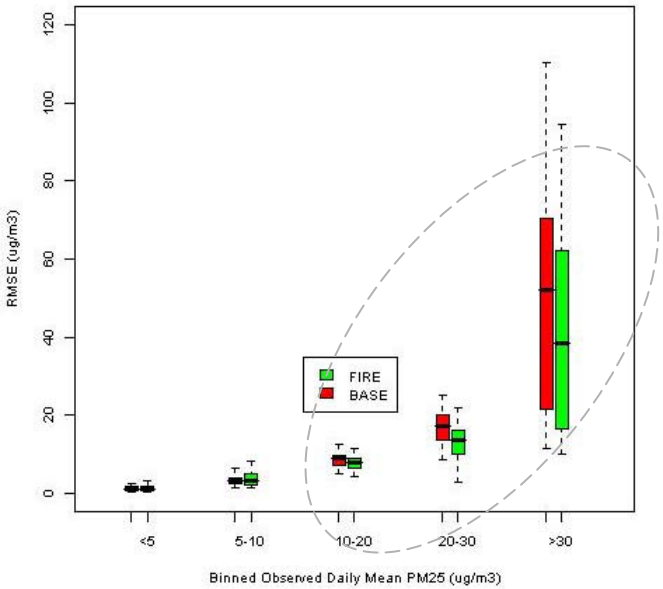




•Reduced Bias

RMSE

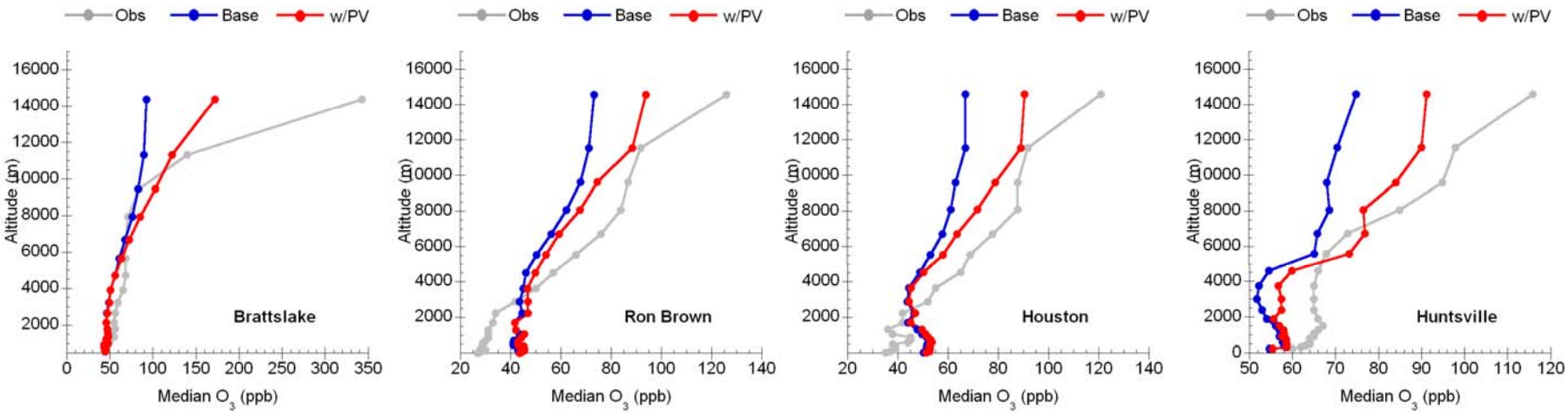




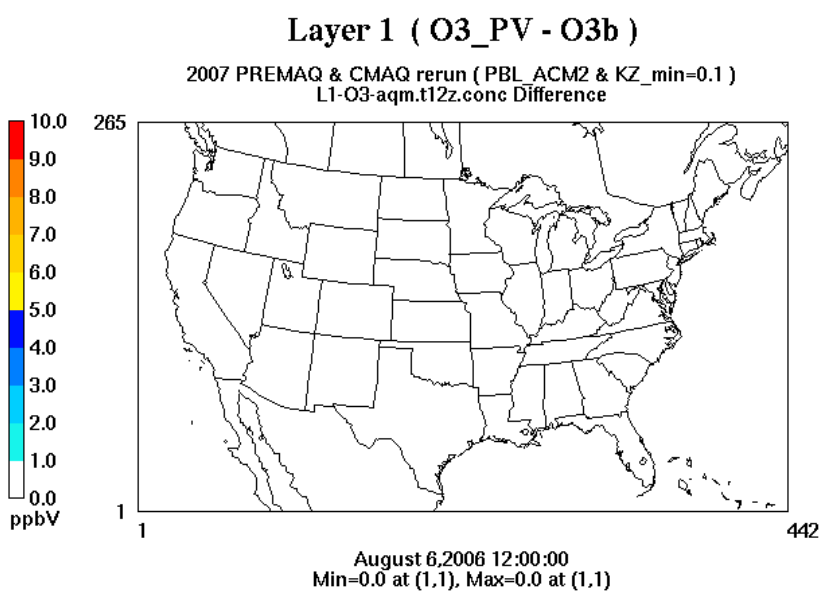
•Reduced Error

Can Use of Potential Vorticity Improve Simulated 3-D O_3 Distribution?

Early Results: Modeled O_3 specified by enforcing proportionality to PV (altitude>8.5km); August 5-29, 2008



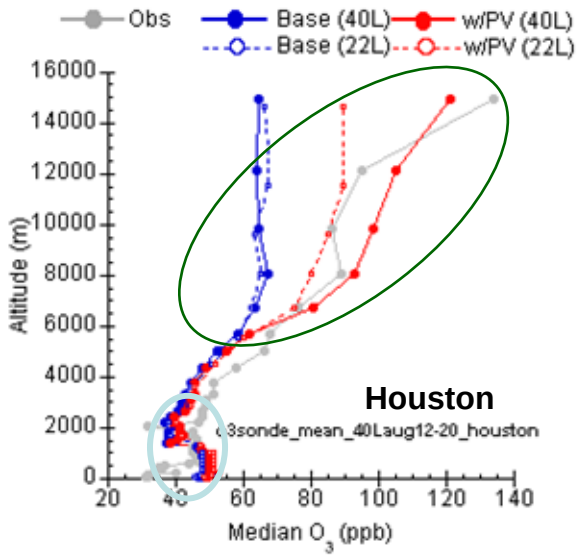
- Improvements in upper and mid-troposphere at all IONS sites
- Improved representation of lower tropospheric values in SE U.S.

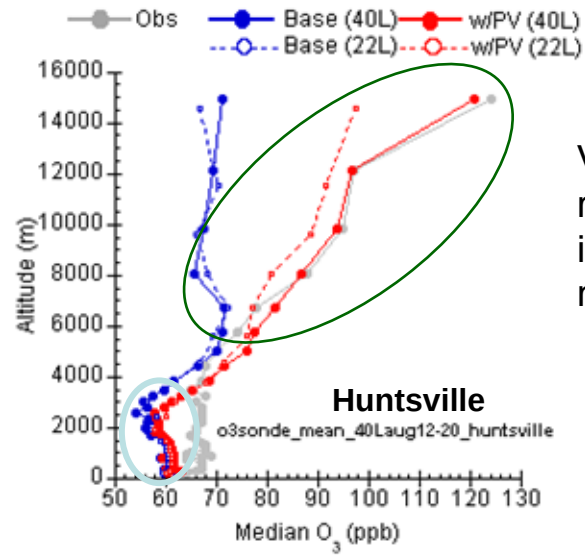


- Enhancements in surface-level O_3 in regions of convective activity and frontal passage

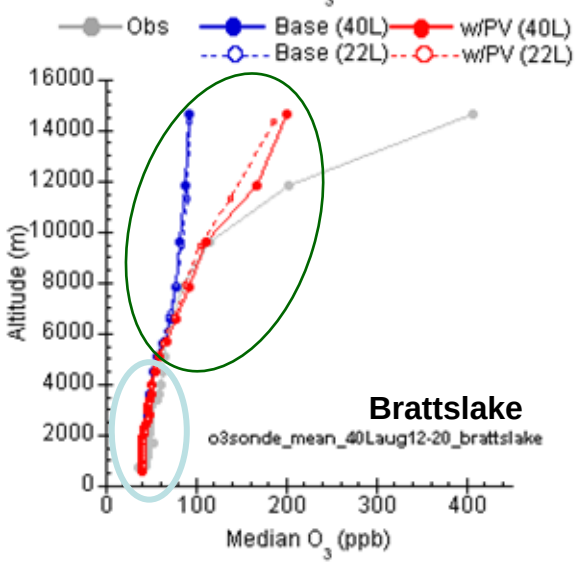
PV and Layer-configuration Tests

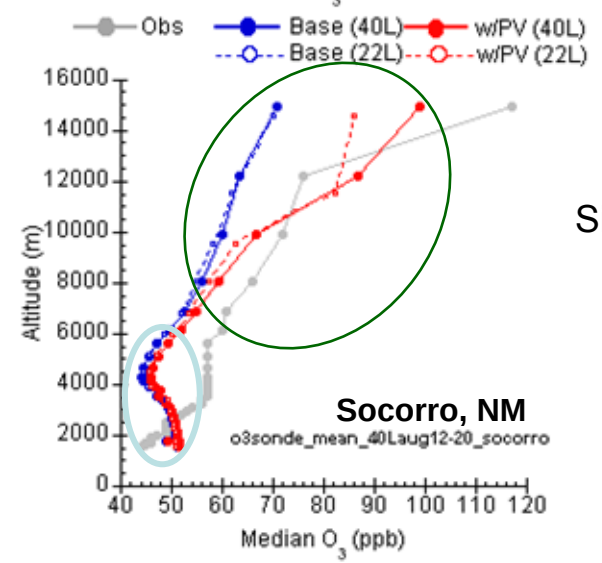
22 and 40 layer CMAQ Configurations





Vertical resolution + PV results in even greater improvement in upper and mid-troposphere

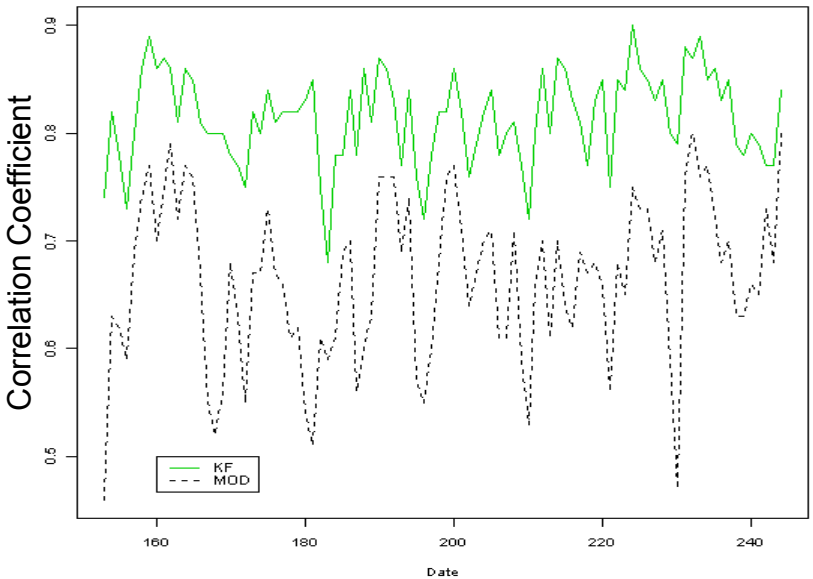


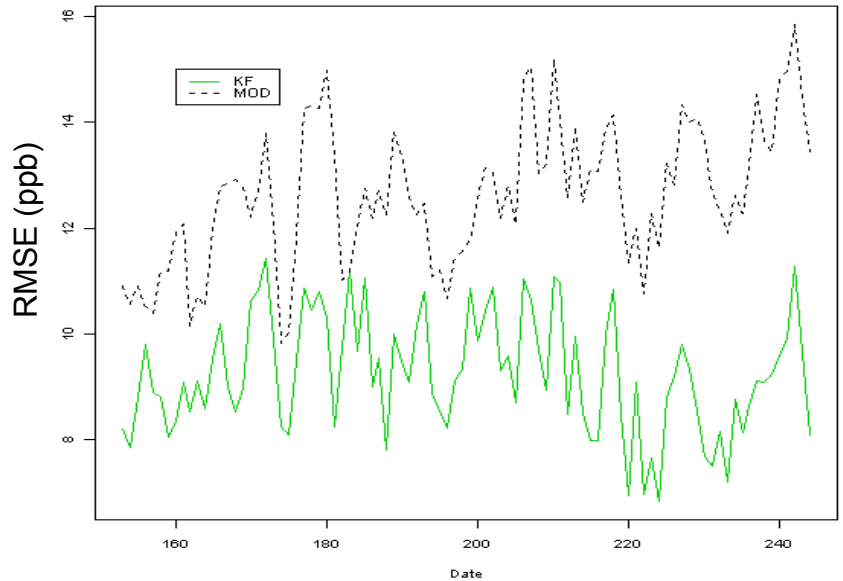


Similar at lower altitudes

Bias Adjustment: Testing in near real-time during 2008

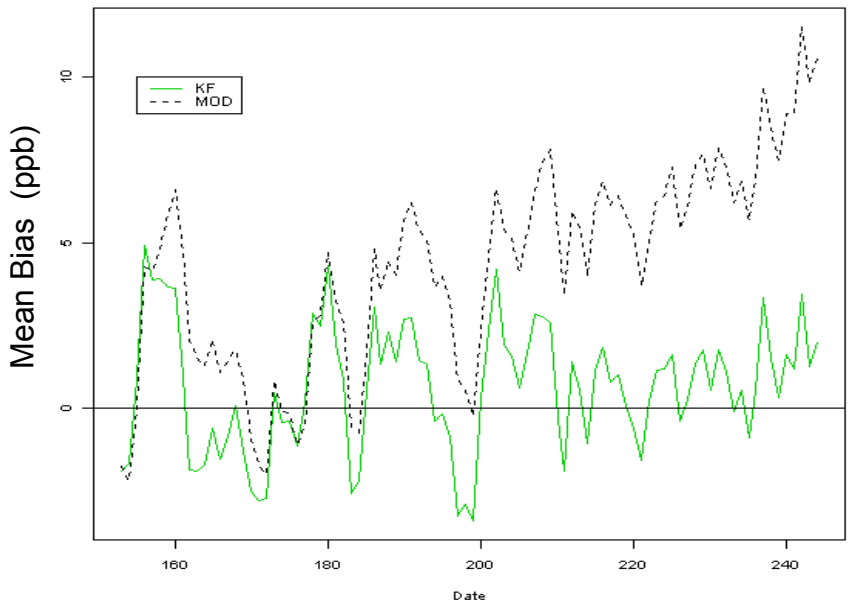
Kalman Filter Predictor Bias Adjustment Method (Kang et al., JGR, in press)





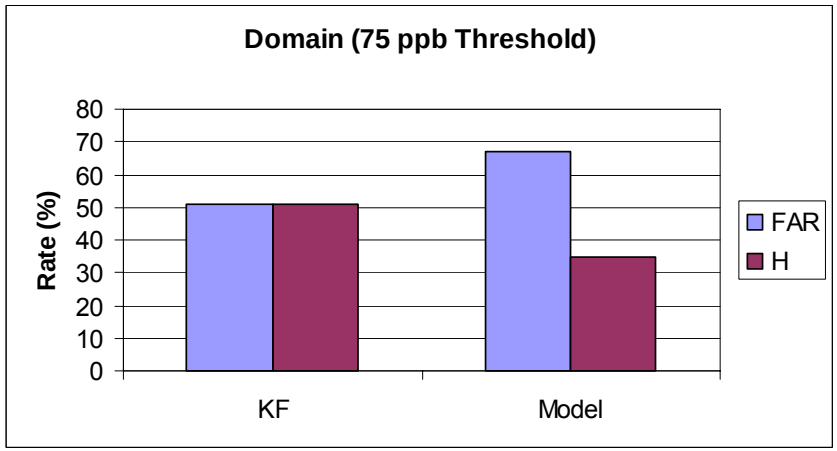
- Statistics across **all CONUS sites**
- June 1 – August 31, 2008

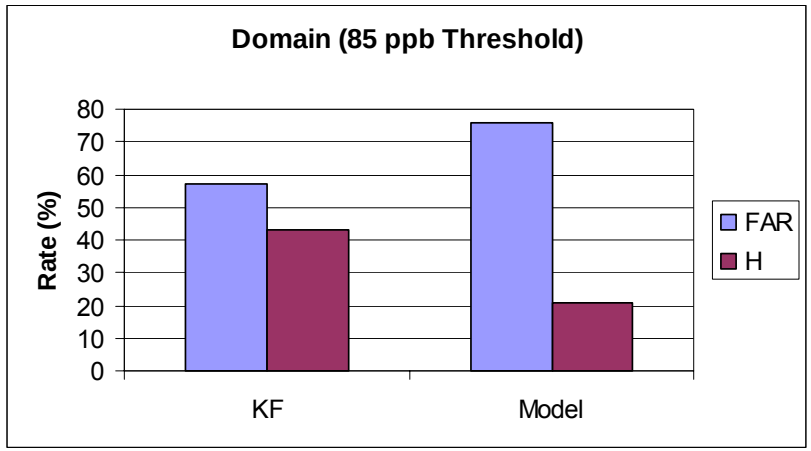
- **Significant improvements in correlation**
- **Significant reduction in bias and error**

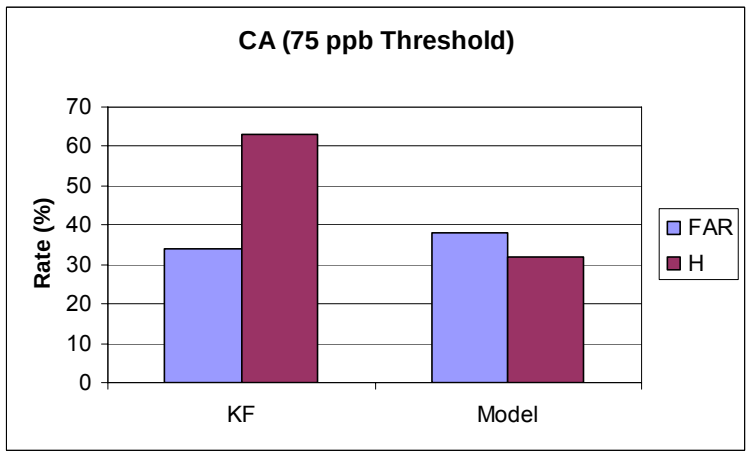


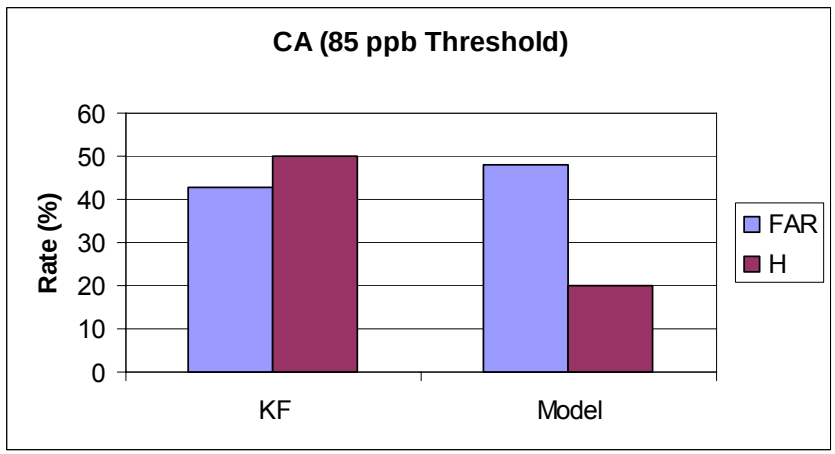
Bias Adjustment: Testing in near real-time during 2008

Categorical Statistics Summary (June-August, 2008)





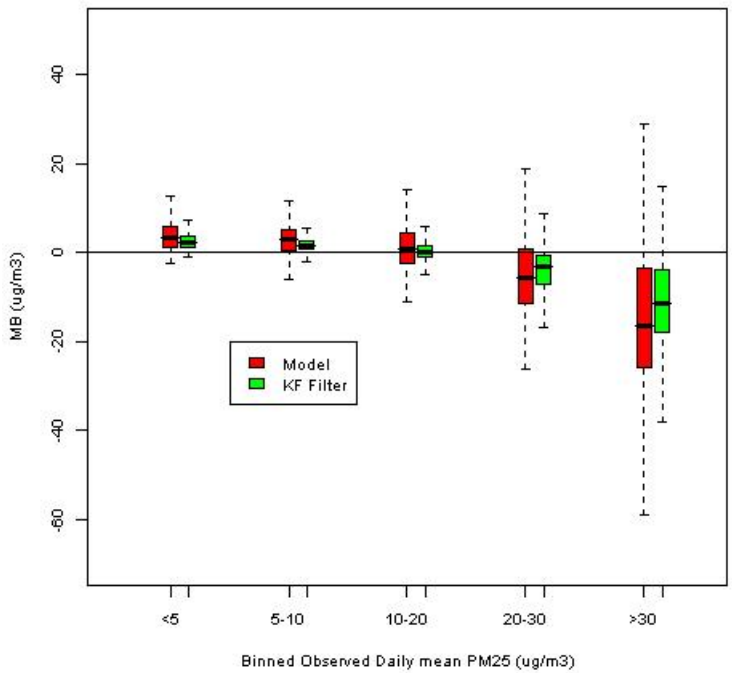


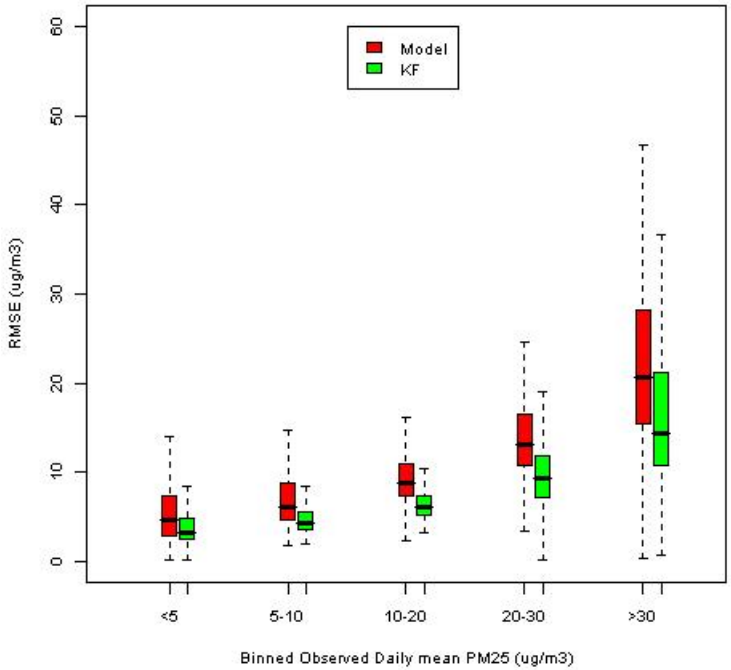


- **Reduces False Alarms**
- **Improves Hit Rate**

Bias Adjustment: Testing in near real-time during 2008

Bias and Errors in $PM_{2.5}$ forecasts (June-August, 2008)

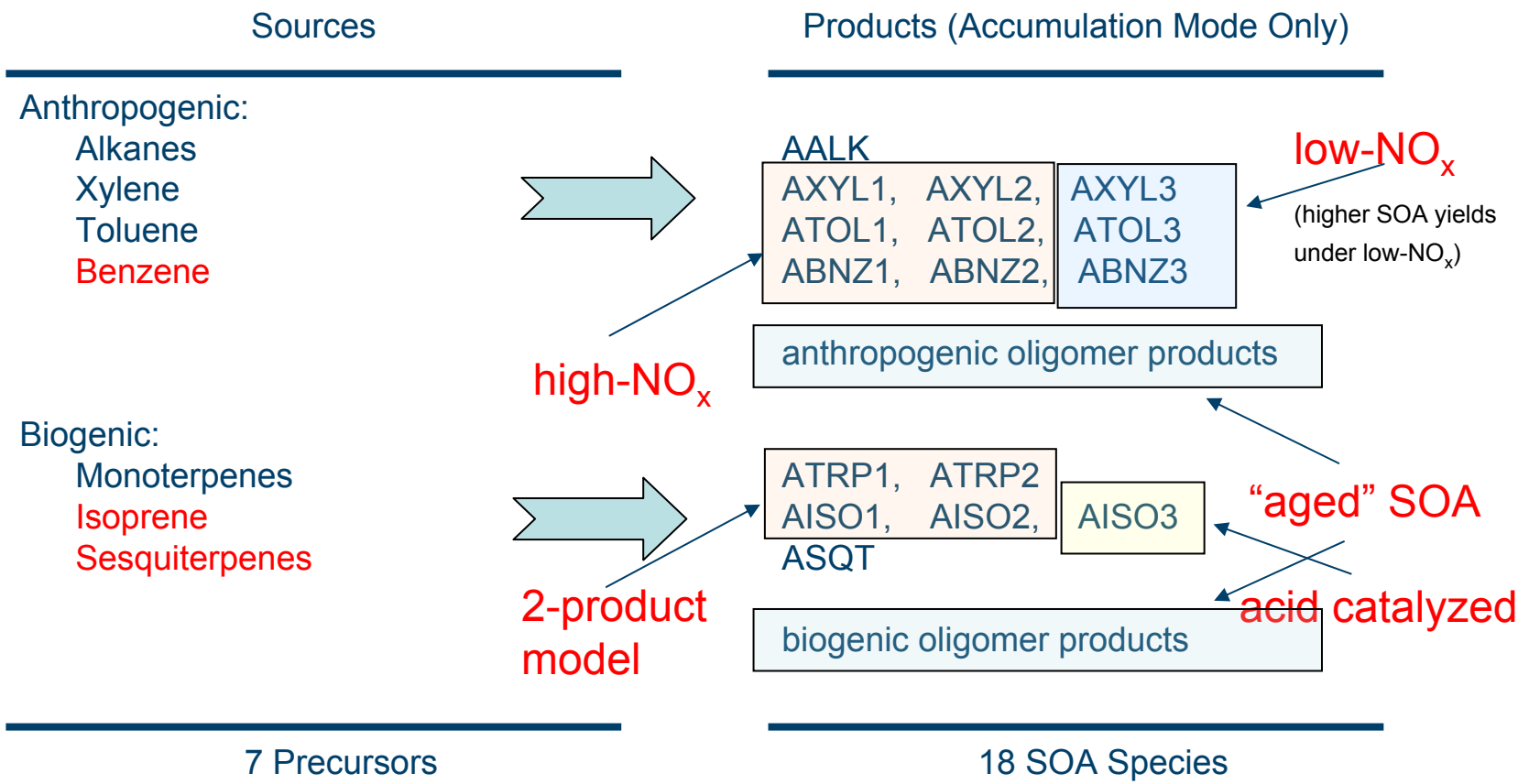




Methodology can also improve $PM_{2.5}$ forecast guidance

Looking Ahead: CMAQv4.7

SOA Formation Pathways in CMAQv4.7



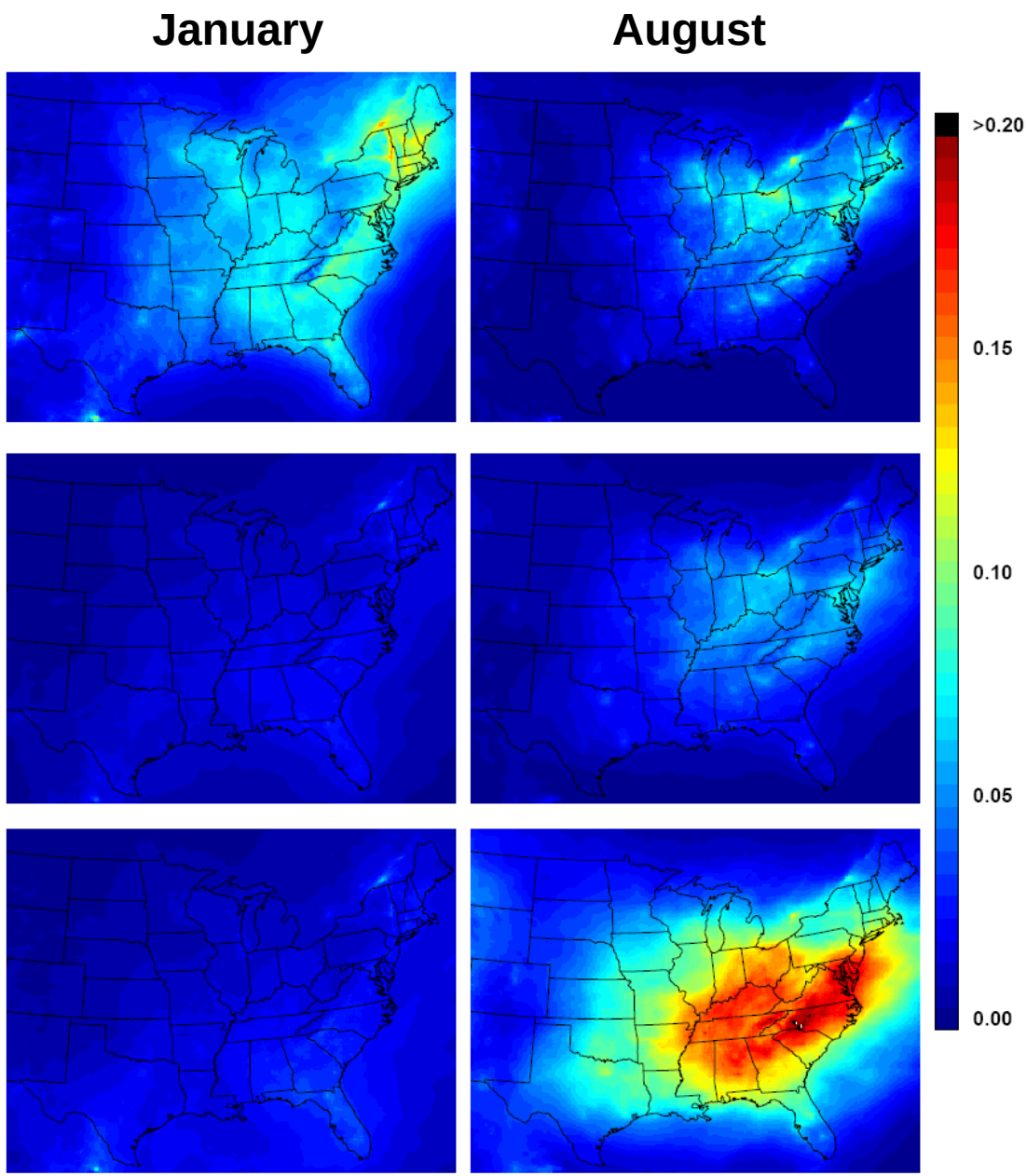
Courtesy: S. Napelenok

Anthropogenic SOA (monthly average, μg/m³)

- **Improves seasonal variability**
- **Summer-time aromatic SOA increase ~ factor of 3**

Change to enthalpy of vaporization

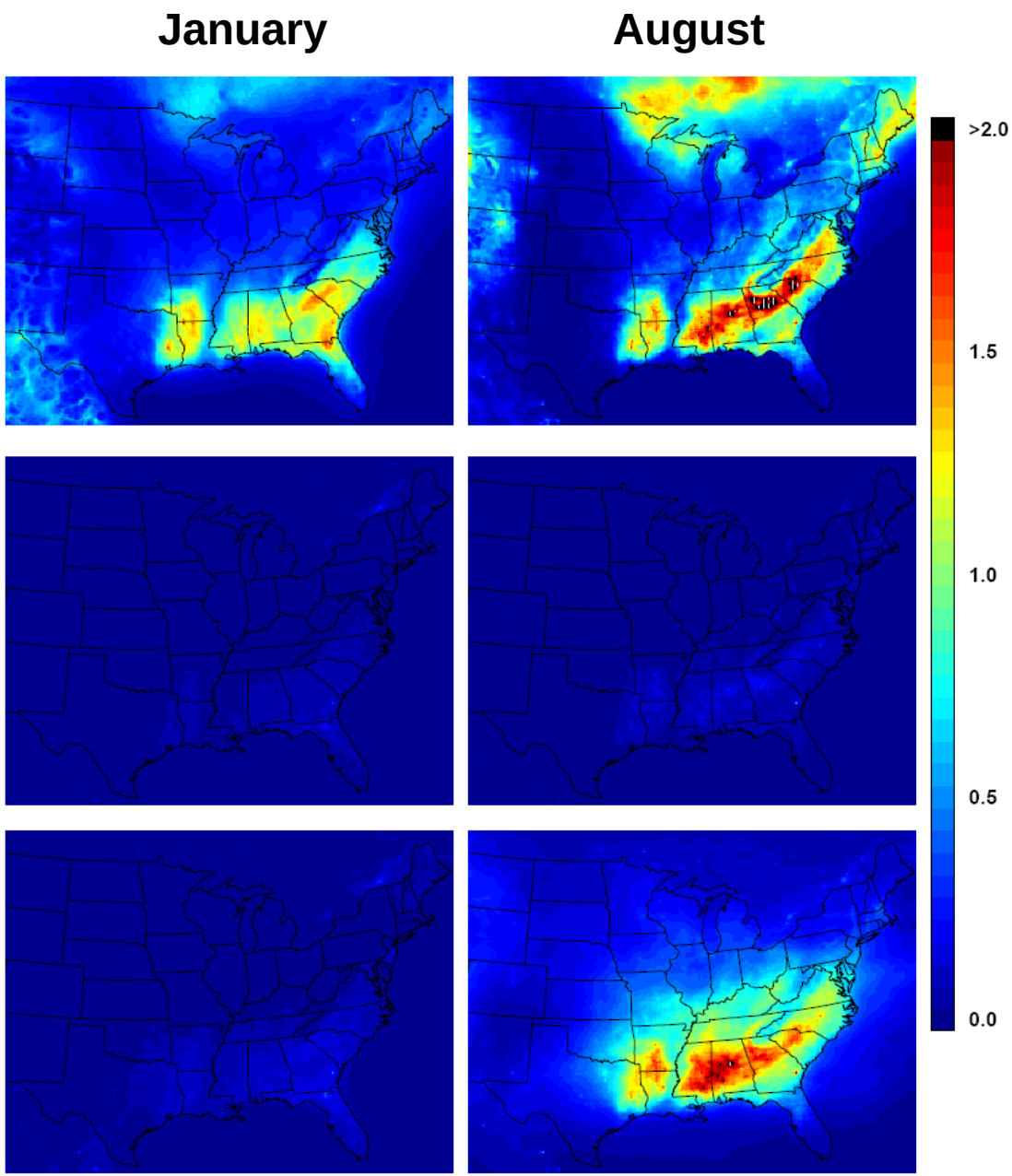
SOA model update



Biogenic SOA (monthly average, µg/m3)

Change to enthalpy of vaporization

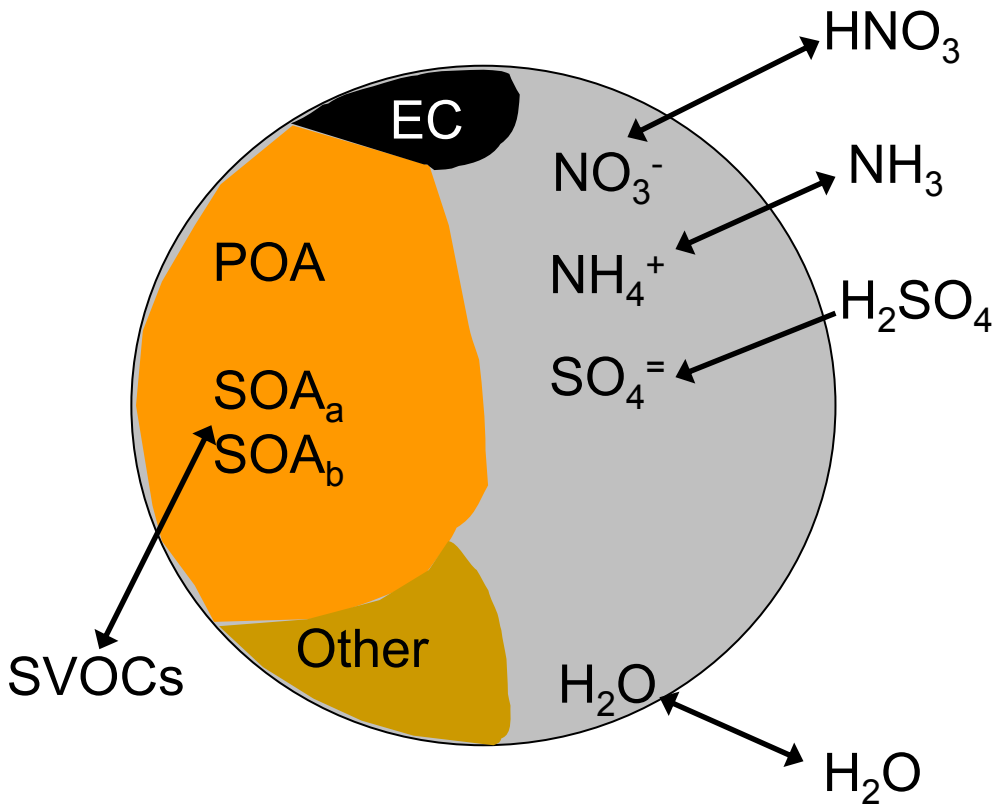
SOA model update



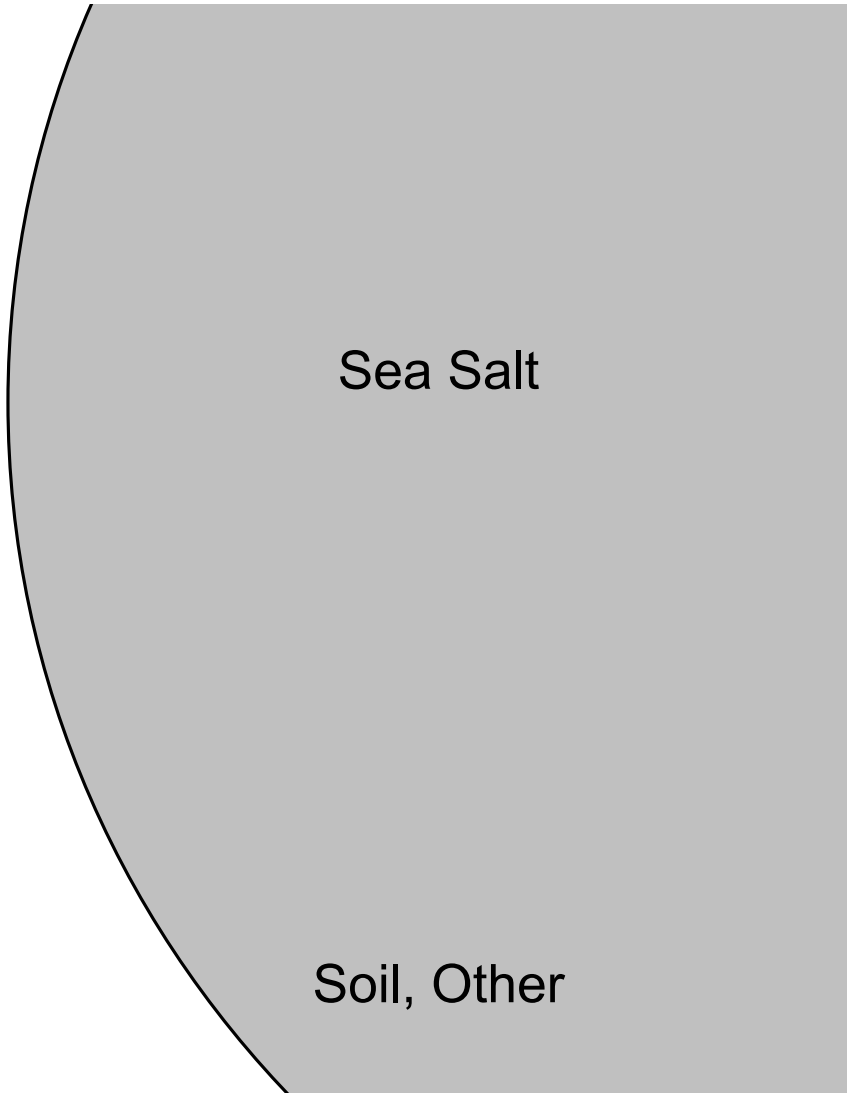
Looking Ahead: CMAQv4.7:

Coarse-mode Chemistry

In current Developmental AQF model:
- Coarse mode is inert.
- Fine mode species equilibrate instantaneously w/ inorganic gases



2 FINE MODES



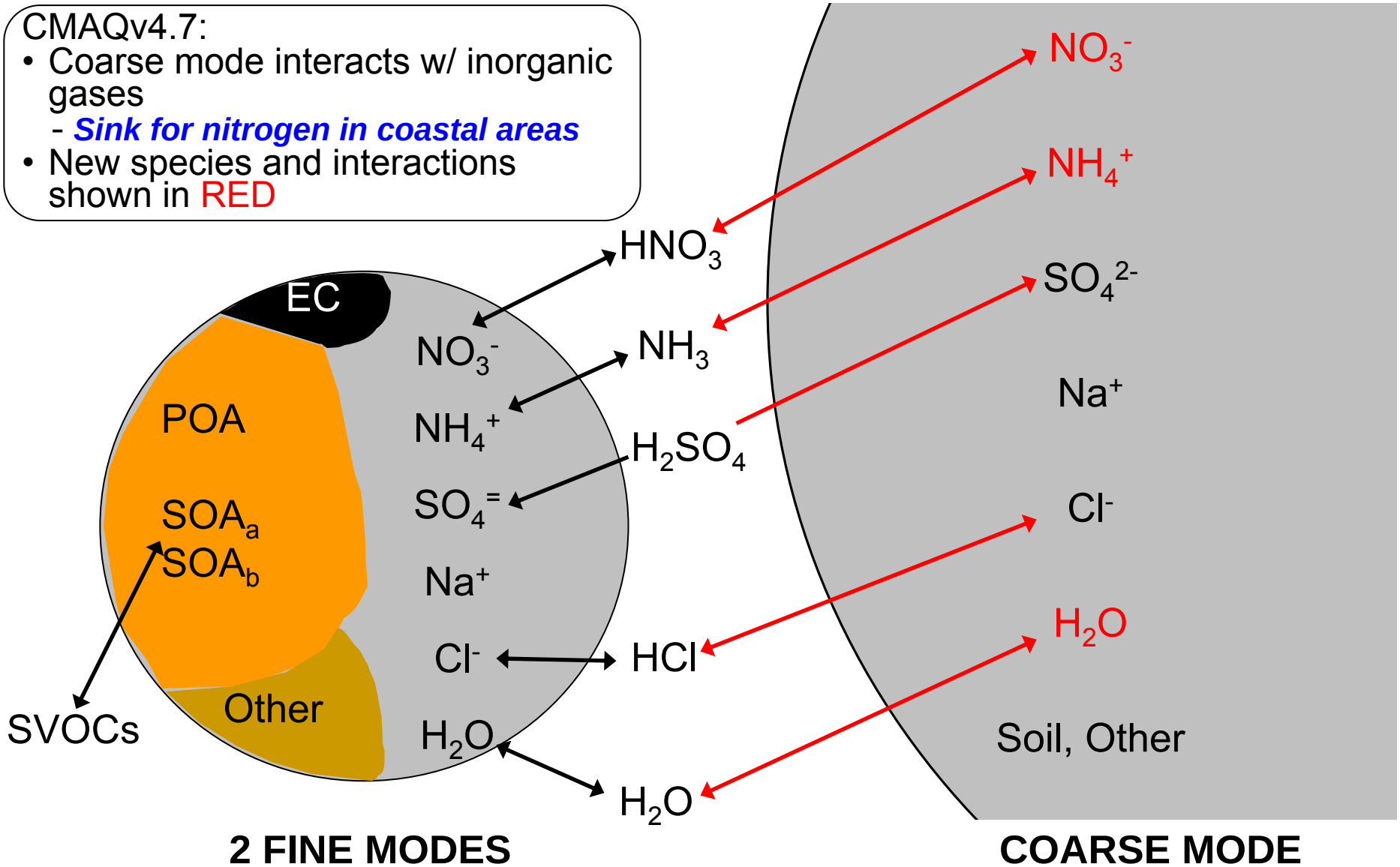
COARSE MODE

Courtesy: P. Bhave

Science Improvements for CMAQv4.7:

Coarse-mode Chemistry

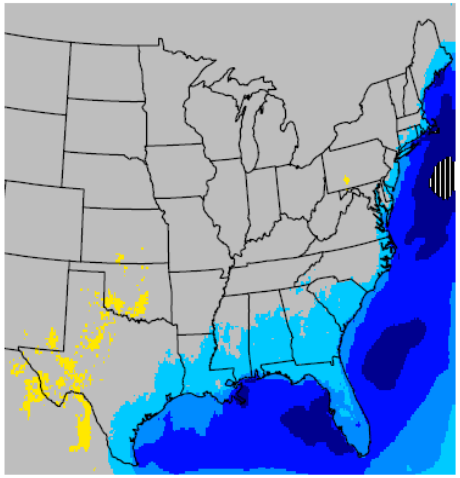
CMAQv4.7:
- Coarse mode interacts w/ inorganic gases
  - ***Sink for nitrogen in coastal areas***
- New species and interactions shown in RED



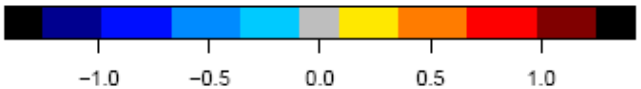
Courtesy: P. Bhave

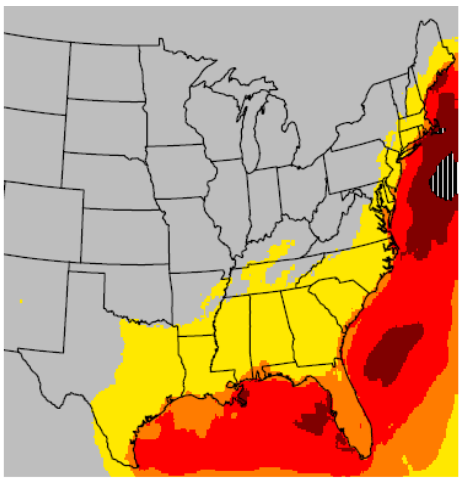
Science Improvements for CMAQv4.7: Coarse-mode Chemistry: Impacts

New vs. Old model average change: January 2006

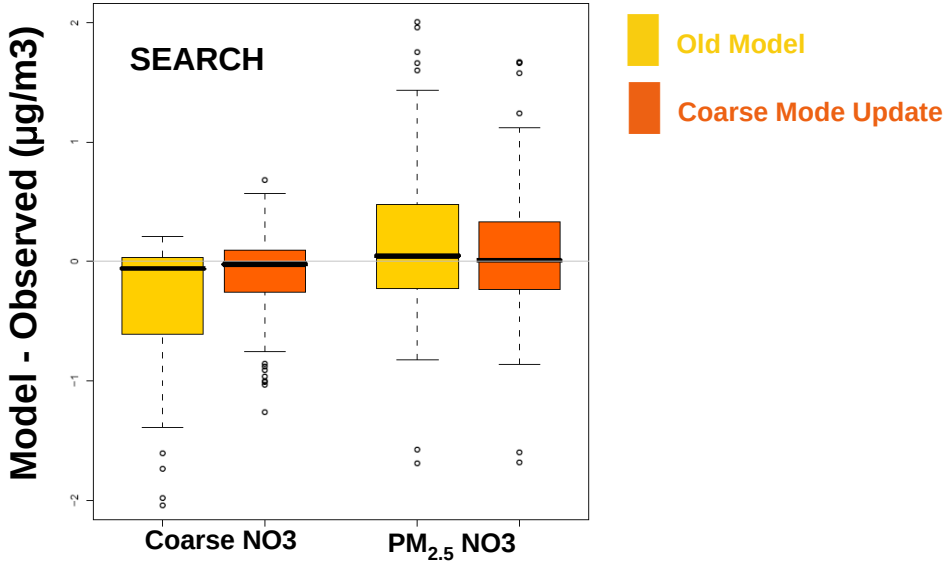


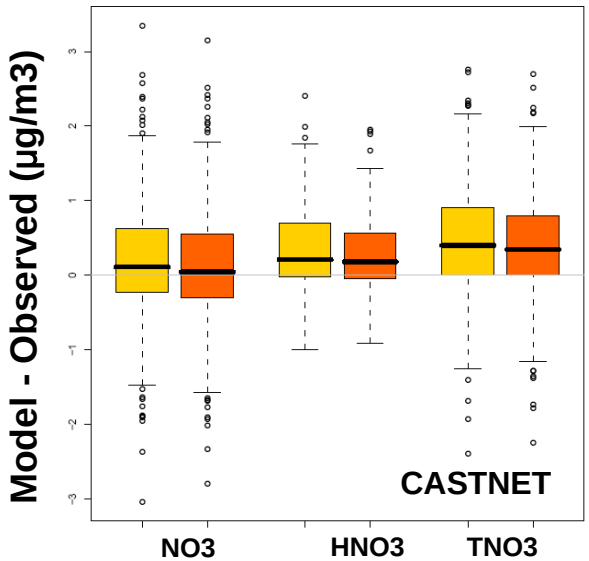
HNO3 (µg/m3) *Decrease*





Coarse NO_3 (µg/m3) *Increase*

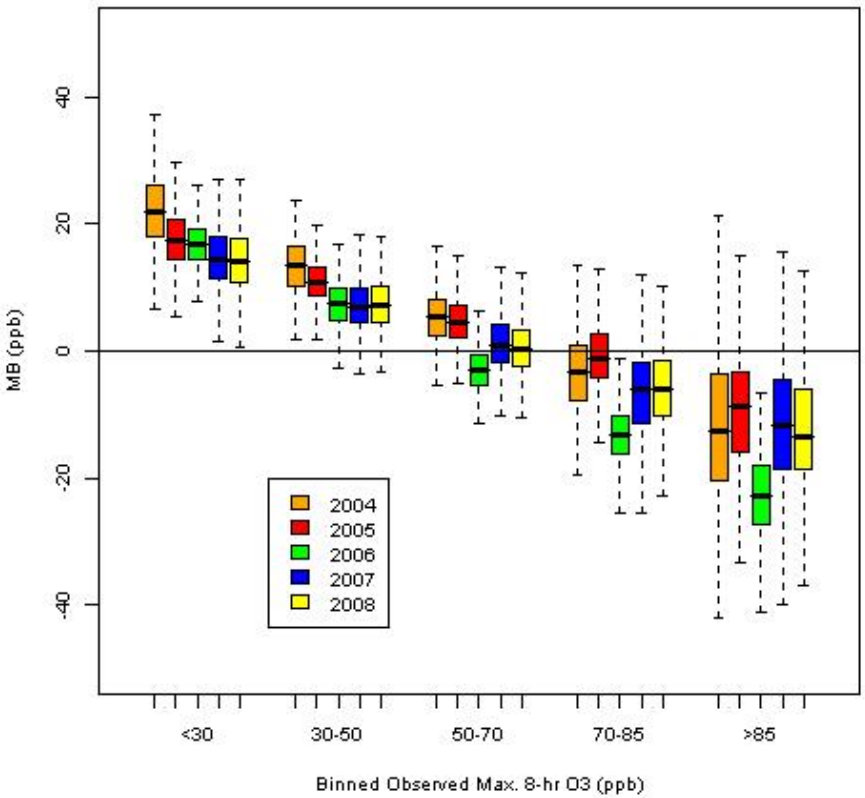


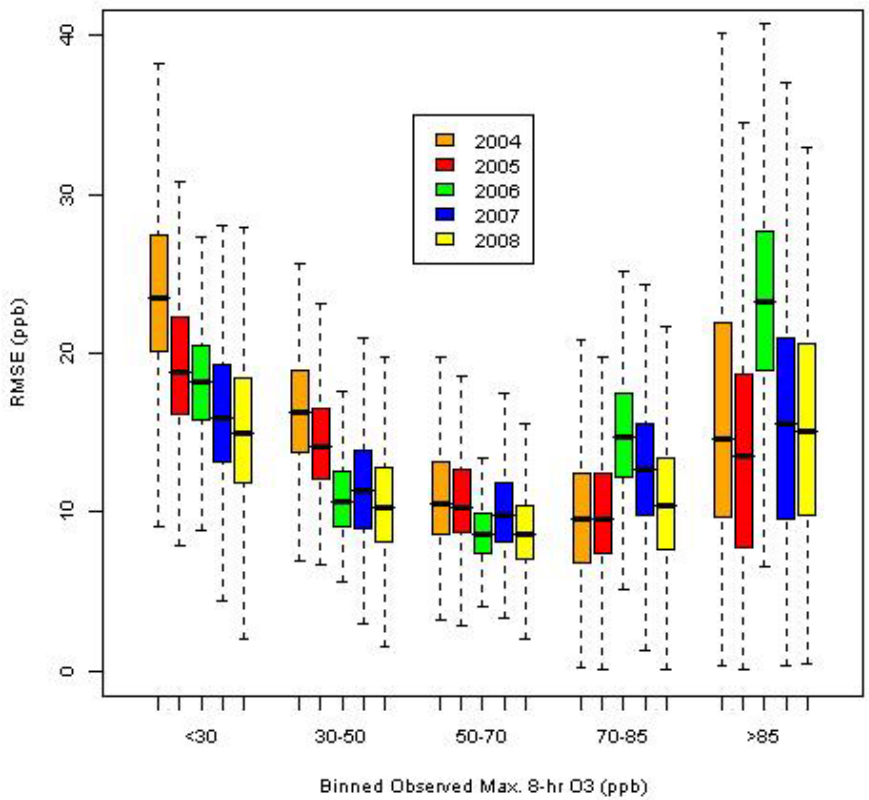


➡ **Accurate representation of partitioning of airborne NO_3 is important for describing transport distances and deposition amounts**

Have model changes resulted in performance improvements?

East U.S. sites, Max 8-hr O_3, operational model predictions





- Continuous improvements in performance over years across most conc. ranges
  - Reduced over-prediction at low concentrations
  - Reduced under-predictions at high concentrations

Summary

- NAM-CMAQ performance for surface-level O_3 forecast guidance has improved continuously during 2004-2008
  - Forecast guidance coverage also continuously expanded
- Though regional statistics with CMAQ-CB05 exhibit higher bias/error compared to CMAQ-CBMIV, CMAQ-CB05 improves "peak prediction" accuracy
  - Lower bias/error at moderate-high observed O_3
  - Regional statistics skewed due to over-prediction at low O_3 range (larger sample)
  - *Transitioning operational system to CB05 recommended*
- Bias-adjustment can improve the accuracy and utility of the model forecast guidance
  - *FY08 testing suggests that implementation in real-time is feasible*
- Incorporation of a methodology for including impacts of wildfires on both O_3 and PM is desirable

……. Its been fun !