THE COMMUNITY MULTISCALE AIR QUALITY (CMAQ) MODEL:

Model Configuration and Enhancements for 2006 Air Quality Forecasting

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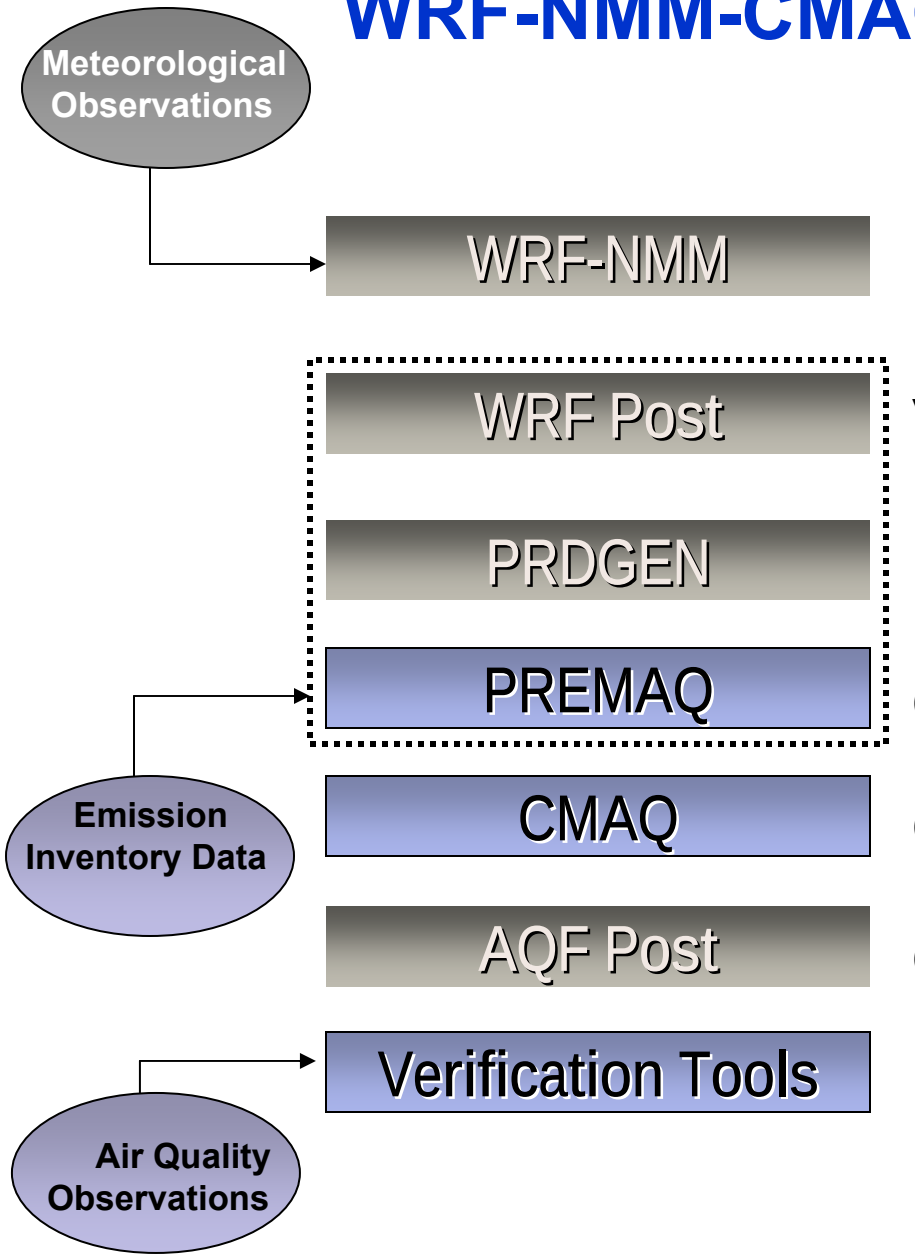
WRF-NMM-CMAQ AQF Capability



NAM Meteorology model

Vertical interpolation

Horizontal interpolation to Lambert grid

CMAQ-ready meteorology and emissions

Chemistry/Transport/Deposition model

Gridded product files for users

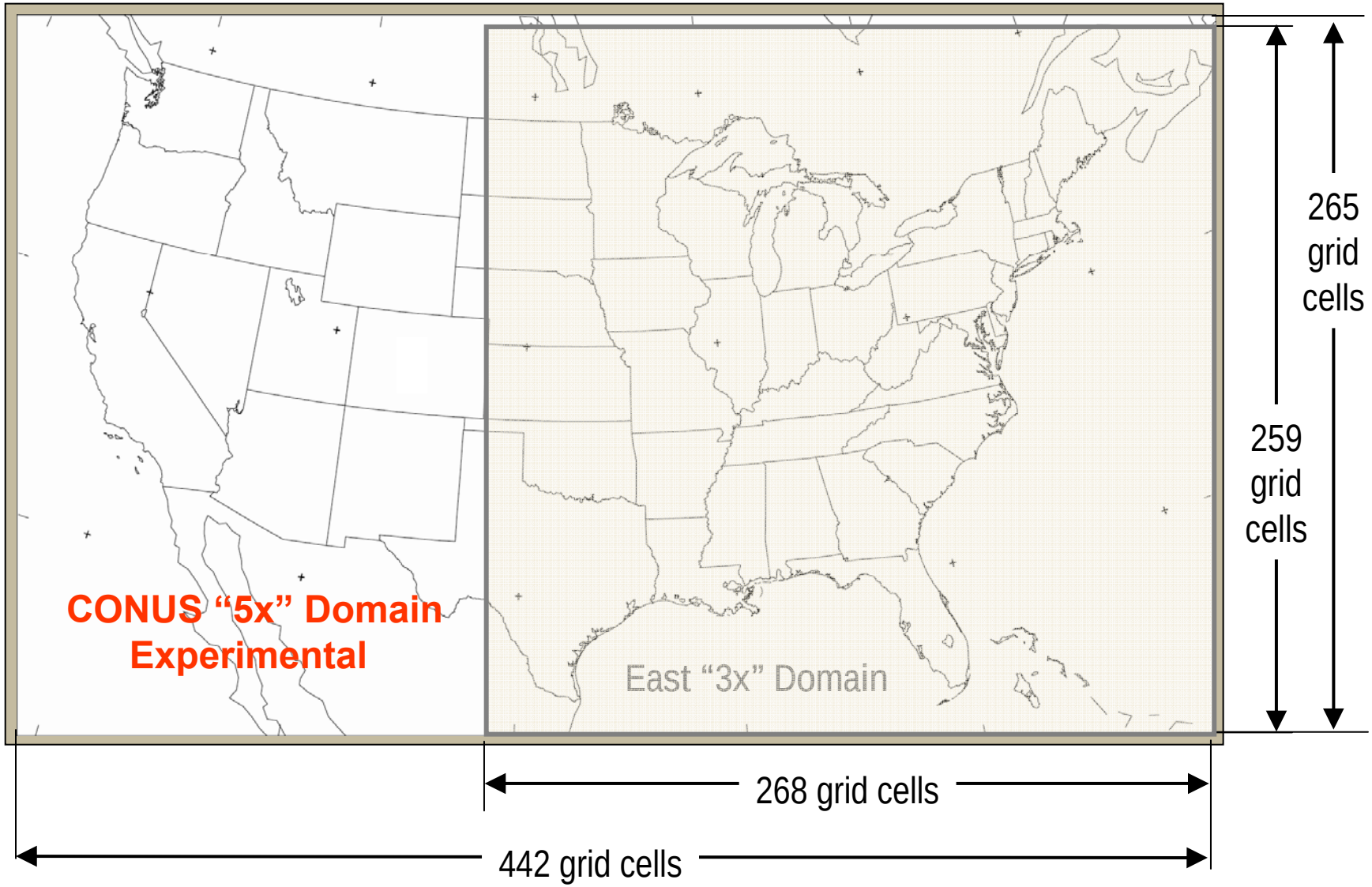
Performance feedback for users/developers

CMAQ Modeling Domains

Experimental PM forecasts on 5x

Ozone forecasts both domains

12 km resolution



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: Computed outside of PREMAQ
  - 2001 NEI version 3 inventory used. (CAIR) No changes made to inventory.
  - Replaced year specific with average (1996-2002) estimates for fires
- Biogenic Sources: BEIS3.13 included directly into PREMAQ.
- Canadian Inventory: 1995 used (includes all provinces)
- Mexican Inventory: BRAVO 1999 used for point sources

Mobile Sources

- SMOKE/MOBILE6 not efficient for real-time forecasting
- SMOKE/MOBILE6 used to create retrospective emissions for AQF grid
  - 2006 (projected from 2001) VMT data used for input to Mobile 6
  - 2006 Vehicle Fleet used for input to Mobile 6
- For 13 counties in Metropolitan Atlanta area, VMT based on 2005 run of a travel demand model and Mobile6 *inputs from Georgia DNR*

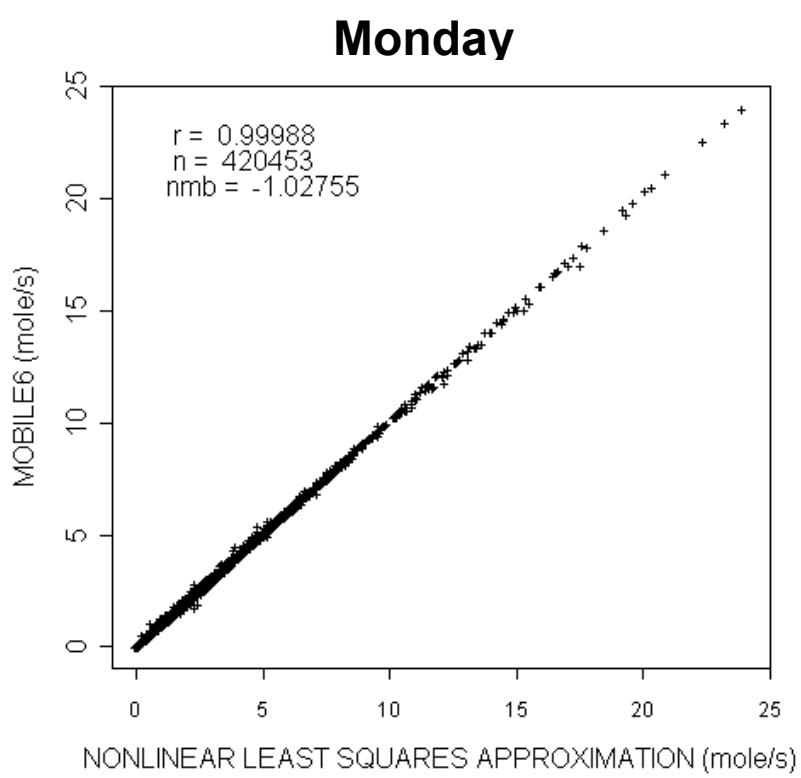
Mobile Sources

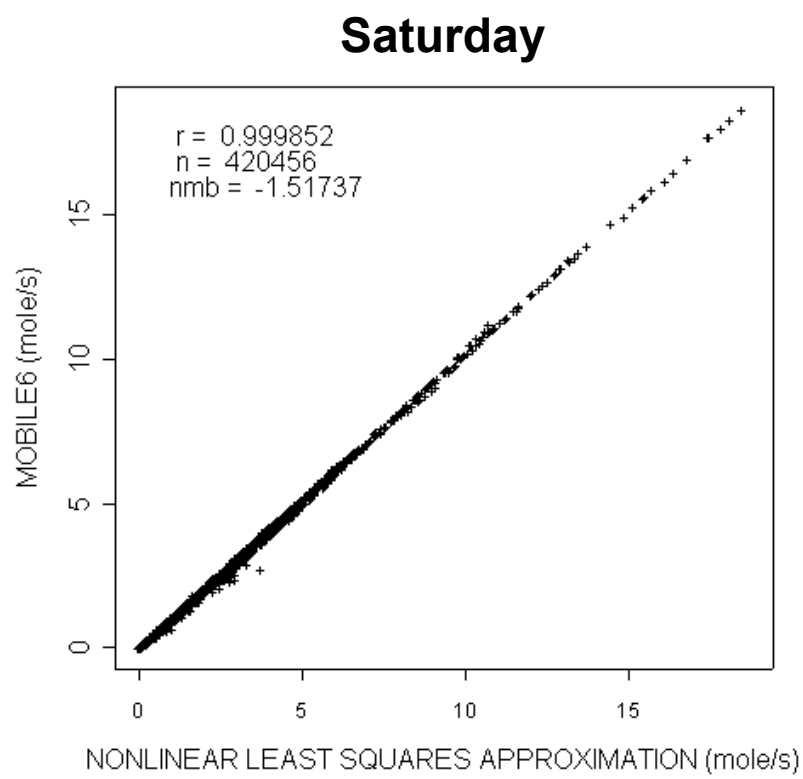
- Regression applied at each grid cell at each hour of the week for each species to create temperature/emission relationship
- Mobile Source emissions calculated in real-time using this derived temperature/emission relationship

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

- For California used 2001 mobile estimates from CARB

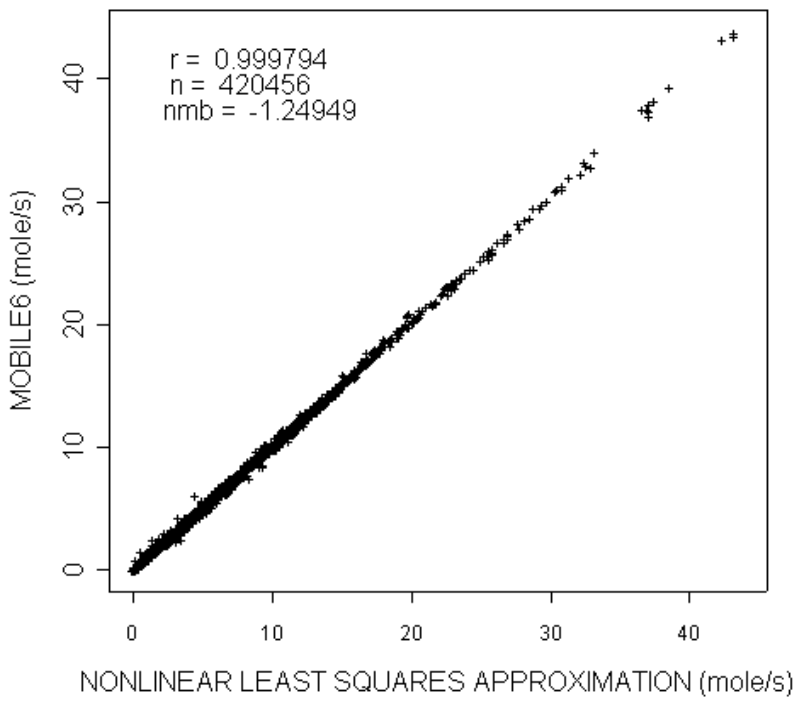
NE Domain Mobile6 vs. Regression: NO_x



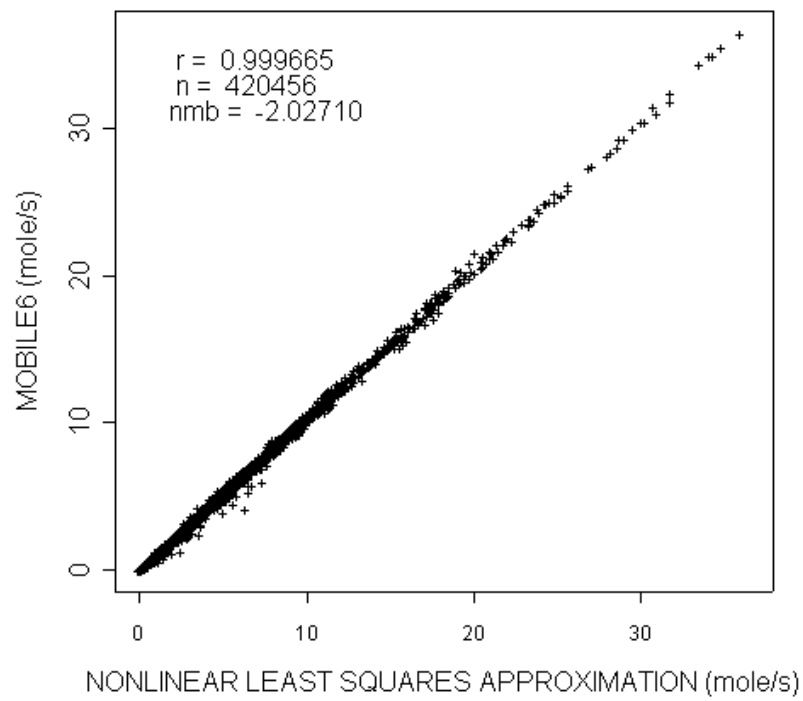


NE Domain Mobile6 vs. Regression: VOC

Monday



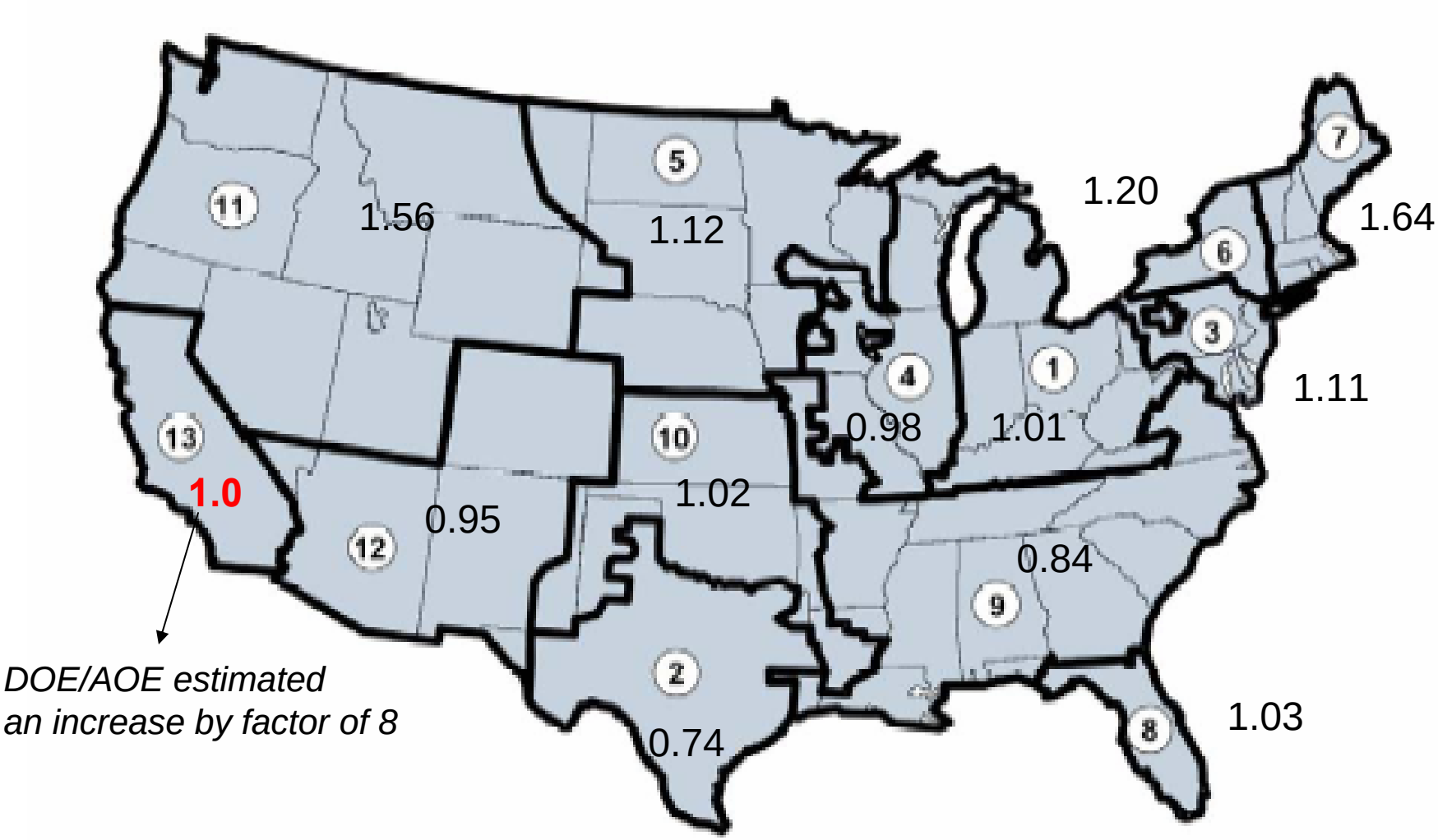
Saturday



Point Sources

- 2004 Continuous Emissions Monitoring for NO_x and SO_2
  - Monthly temporal profiles on a state-by-state basis derived from 2004 CEM
- For other pollutants and non-EGU: 2001 NEIv3
  - Georgia non-EGU based on 2002 inventory from GADNR
- Modified EGU NOx emissions using DOE's Annual Energy Outlook (Jan. 2006)
- Calculated 2006/2004 NO_x and SO_2 annual emission ratios on a regional basis (from DOE data)
  - *Exception California*

EGU NO_X adjustments 2006/2004 by region



Source: Department of Energy Annual Energy Outlook 2006

http://www.eia.doe.gov/oiaf/aeo/index.html

CMAQ Configuration

- **Advection**
  - Horizontal: *Piecewise Parabolic Method*
  - Vertical: *Upstream with rediagnosed vertical velocity to satisfy mass conservation*
- **Turbulent Mixing**
  - K-theory; PBL height from WRF-NMM
  - 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

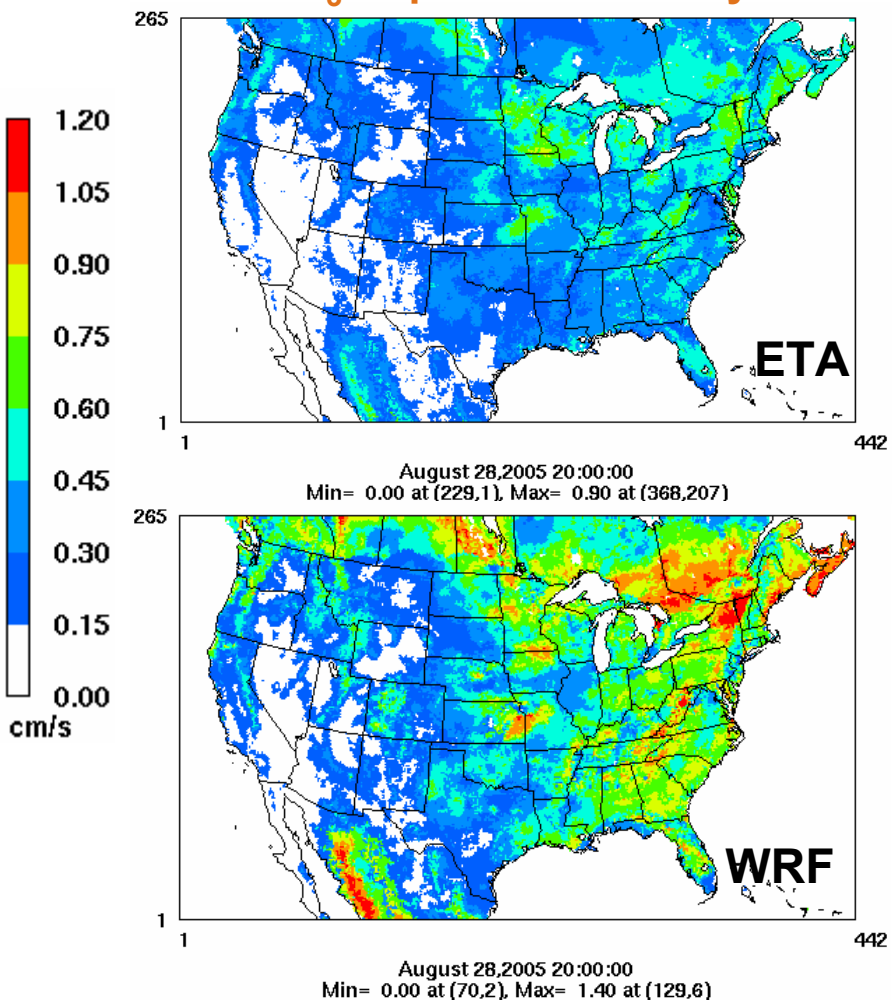
CMAQ Configuration (contd.)

- **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 the NAM fields
- **Cloud Processes**
  - Mixing and aqueous chemistry
  - Scavenging and wet deposition
  - Sub-grid scheme based on modifications to RADM formulation; "switch-off" entrainment from above clouds
    - **Used in Eastern U.S. (3x) domain**
  - "In-cloud" mixing based on the Asymmetric Convective Mixing (ACM) model (Pleim and Chang, 1992, *JGR*)
    - **Used in Continental U.S. (5x) domain**

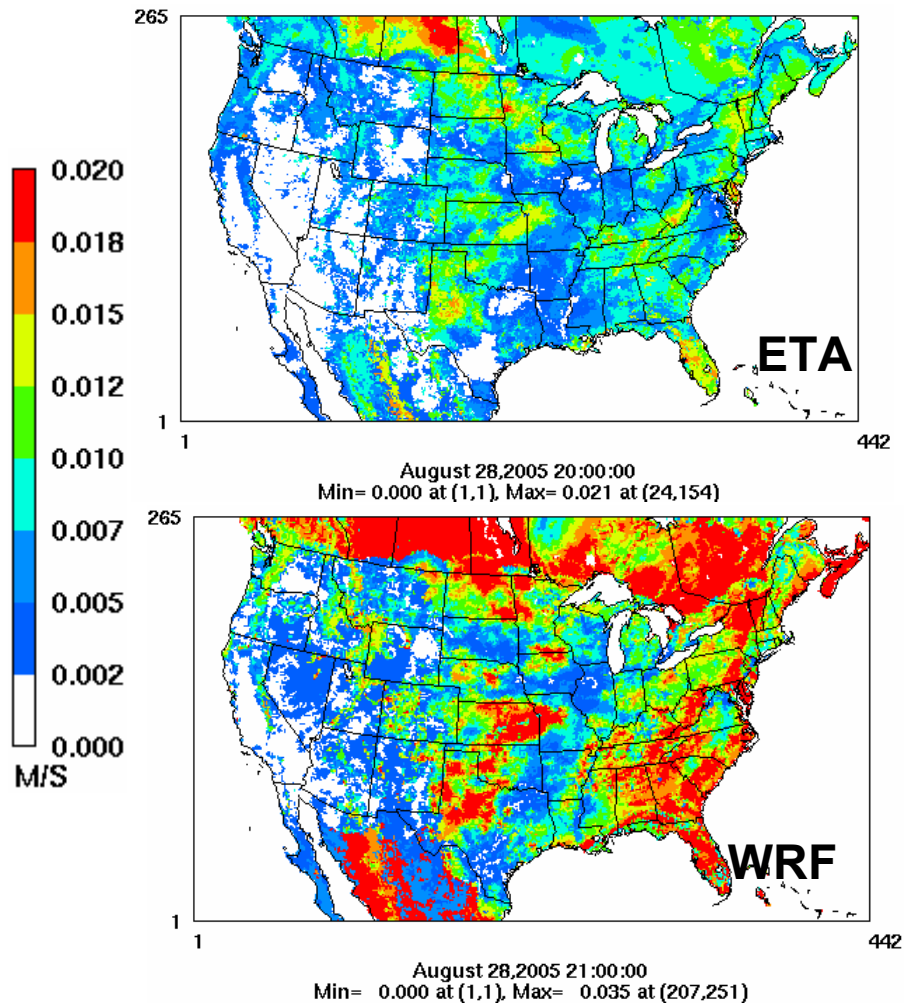
CMAQ Configuration (contd.)

- **Deposition**
  - Dry : M3dry modified to use WRF land surface parameters
  - Changes in WRF-LSM impact V_{do3} (relative to Eta)
    - Persistent sink for O3 – can impact predicted O_3

O_3 Deposition Velocity



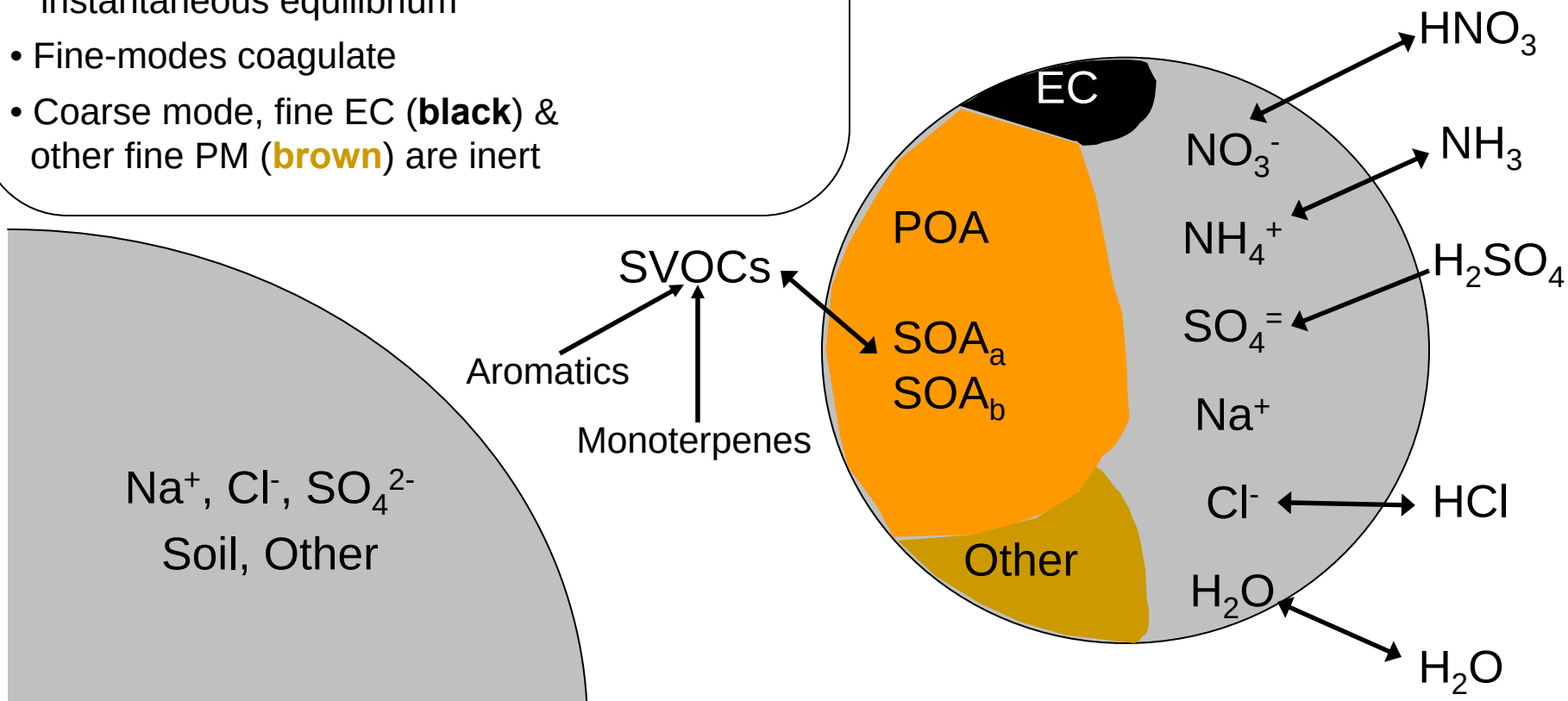
Stomatal Conductance



CMAQ Configuration: Aerosols

- Trimodal size distribution
- Aitken (0-0.1 µm), Accumulation(0.1-2.5 µm), and Coarse
- Gas/particle interactions treated for fine modes only – ISORROPIA instantaneous equilibrium
- Fine-modes coagulate
- Coarse mode, fine EC (**black**) & other fine PM (**brown**) are inert

Binkowski and Roselle, JGR, 2002



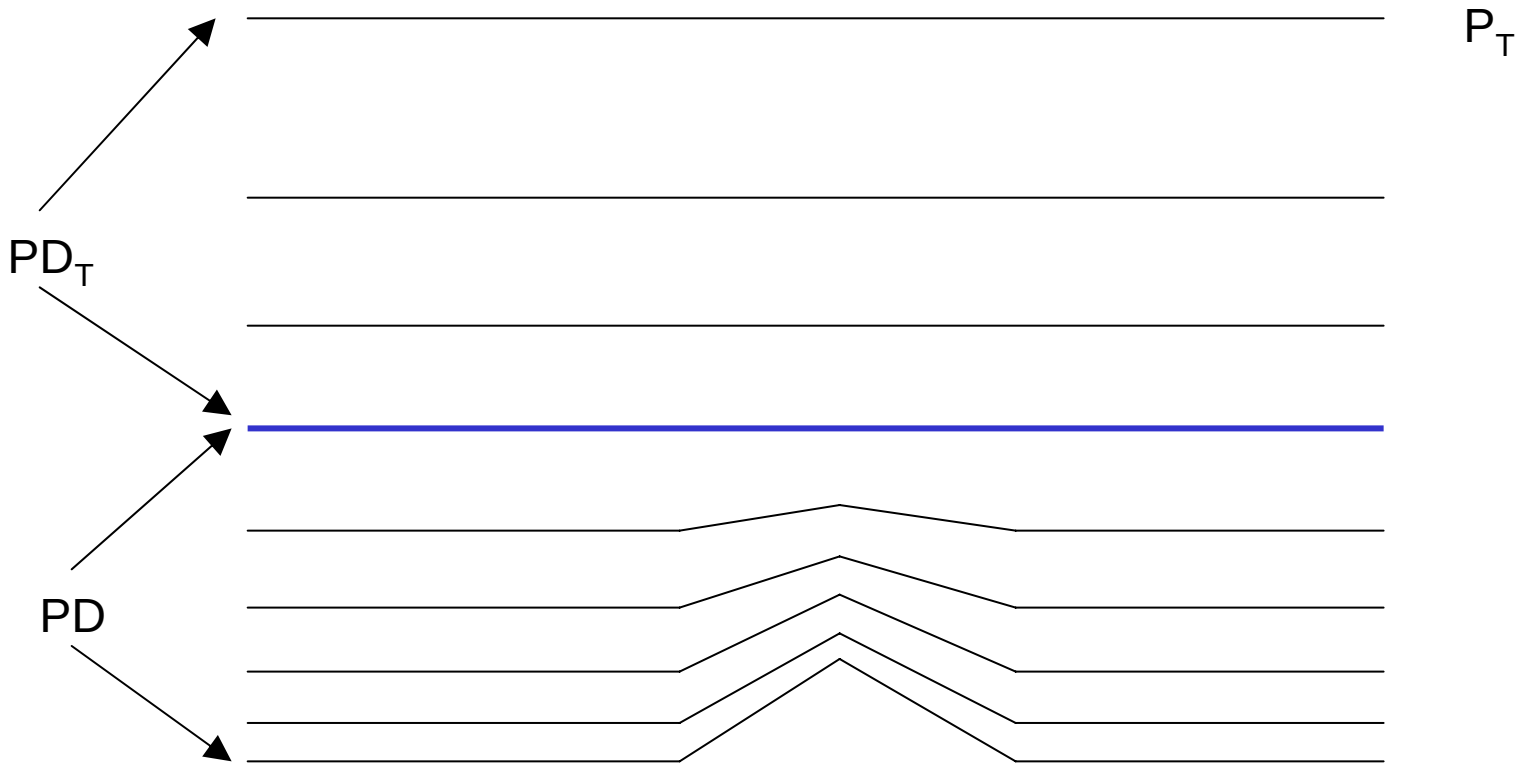
COARSE MODE

2 FINE MODES

Structural Enhancements

- Included layer dependent advection time-step calculation
  - Improves model efficiency
- Coupling between WRF-NMM and CMAQ
  - "**Loose-coupling**" (*used in Operational 3X*)
    - Similar to previous Eta-CMAQ linkage
    - WRF-NMM and CMAQ coordinate and grid structures are different. Interpolation of meteorological inputs to the CMAQ grid and coordinate
  - "**Tight-coupling**" (*implemented in Experimental 5X*)
    - Step 1: Coupling in the vertical implemented this summer
      - CMAQ calculations on the same vertical coordinate as WRF-NMM
    - Step 2: Modifications to CMAQ to facilitate *calculations on native WRF-NMM horizontal grid*
      - Stay tuned

WRF-NMM Hybrid Vertical Coordinate System "Tightly Coupled"



$$P_s = PD + PD_T + P_T$$

Tightly Coupled System

Conversion to use WRF-NMM vertical coordinate in PREMAQ and CMAQ

$$P = PD\sigma_1 + PD_T\sigma_2 + P_T$$

$$\sigma_1 = \frac{P - (PD_T + P_T)}{PD}, \sigma_2 = \frac{P - P_T}{PD_T}$$

σ's limited to 0-1

$$x_3 = \frac{(1-\sigma_1) + (1-\sigma_2)}{2}$$

$$J = \frac{\partial z}{\partial x_3}$$

Jacobian: encapsulates coordinate transformations between physical and computational space

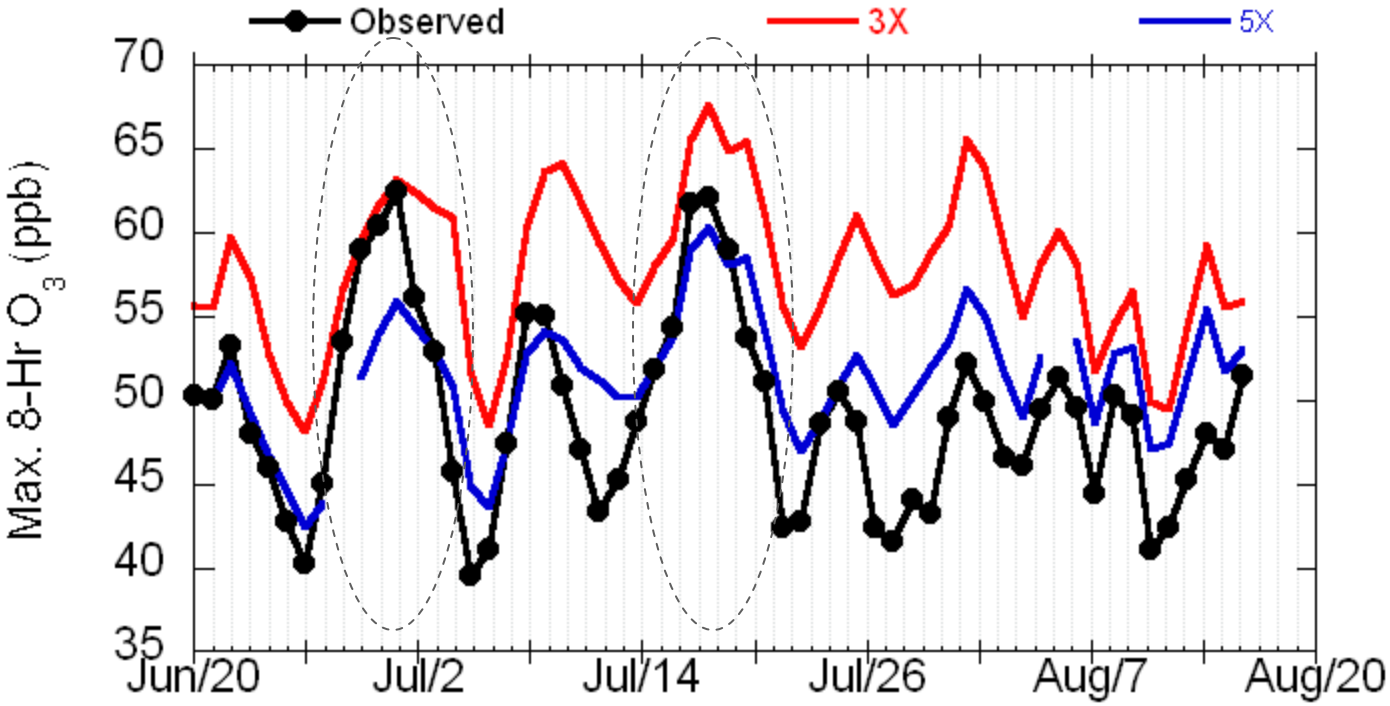
$$J_1 = \frac{2PD}{\rho g}, J_2 = \frac{2PD_T}{\rho g}$$

$$J_h = \frac{(\Delta x_3)_1 J_1 + (\Delta x_3)_2 J_2}{\left[(\Delta x_3)_1 + (\Delta x_3)_2\right]}$$

Jacobian across the interface

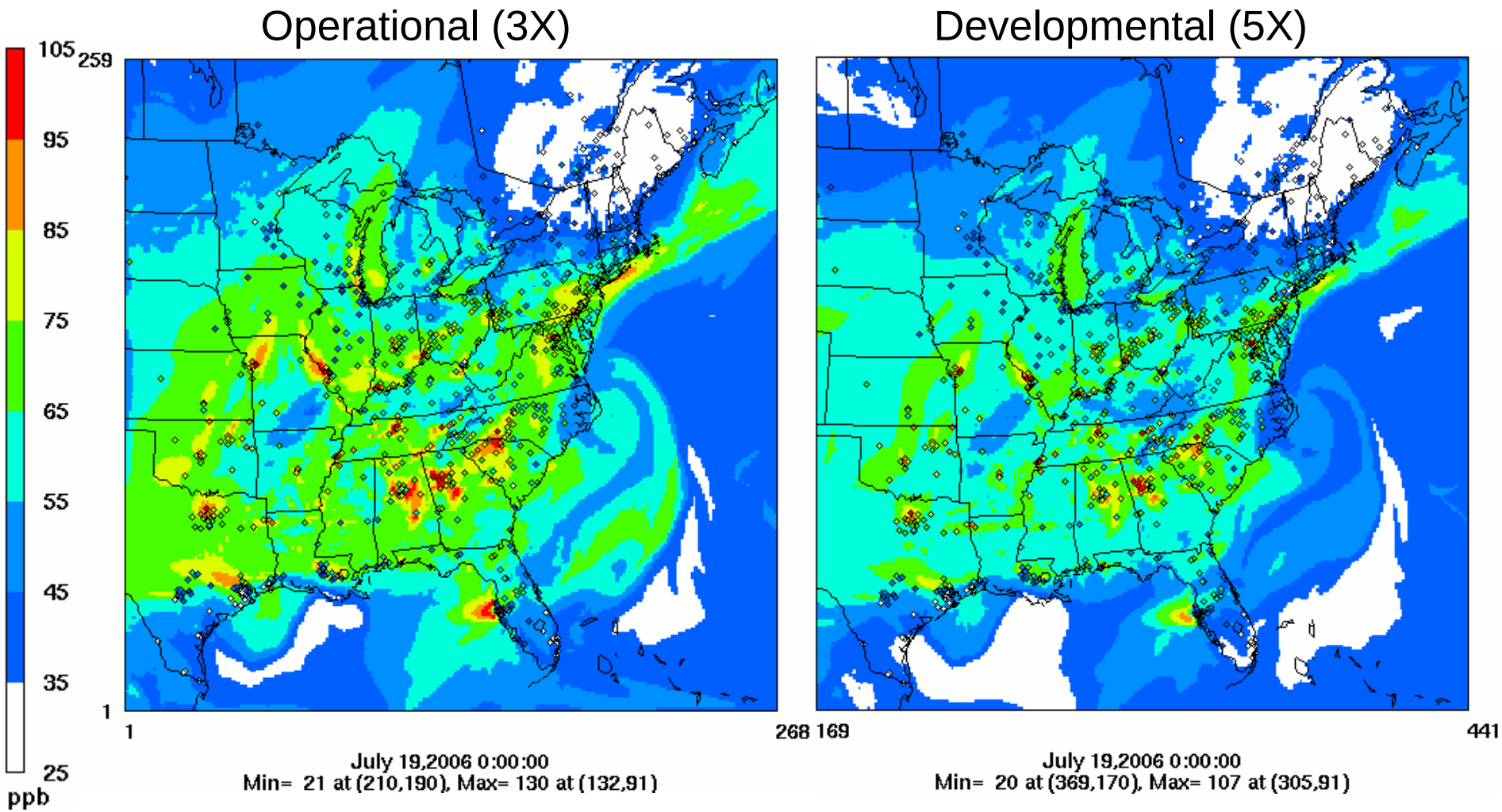
Comparison of Experimental and Operational Forecasts

Mean over sites within Operational 3x Domain



5X under-predictions at peak values

Comparison of Experimental and Operational Forecasts

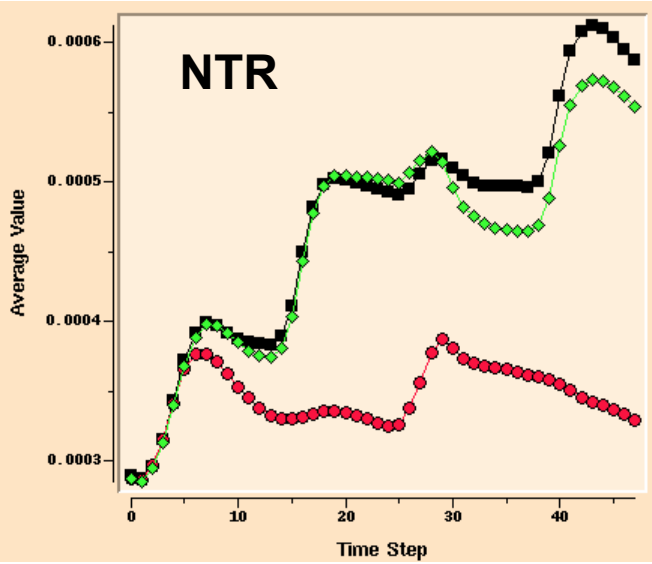


5X vs. 3X: Regionally lower O_3; under-prediction of peak values

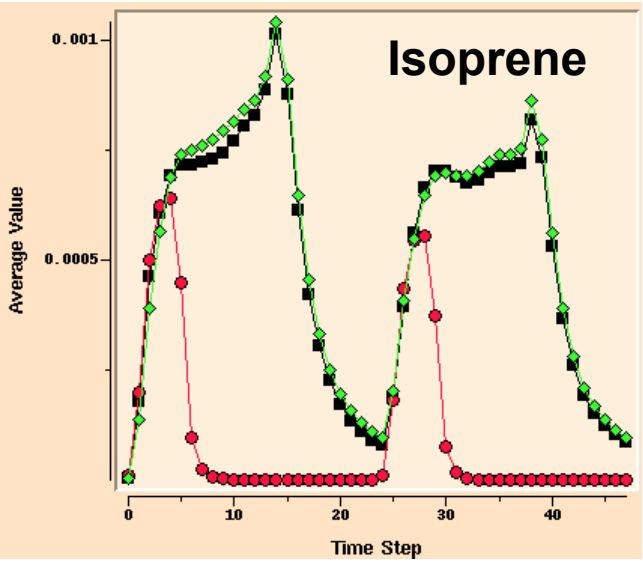
Diagnosing the low-bias in Experimental 5X Runs

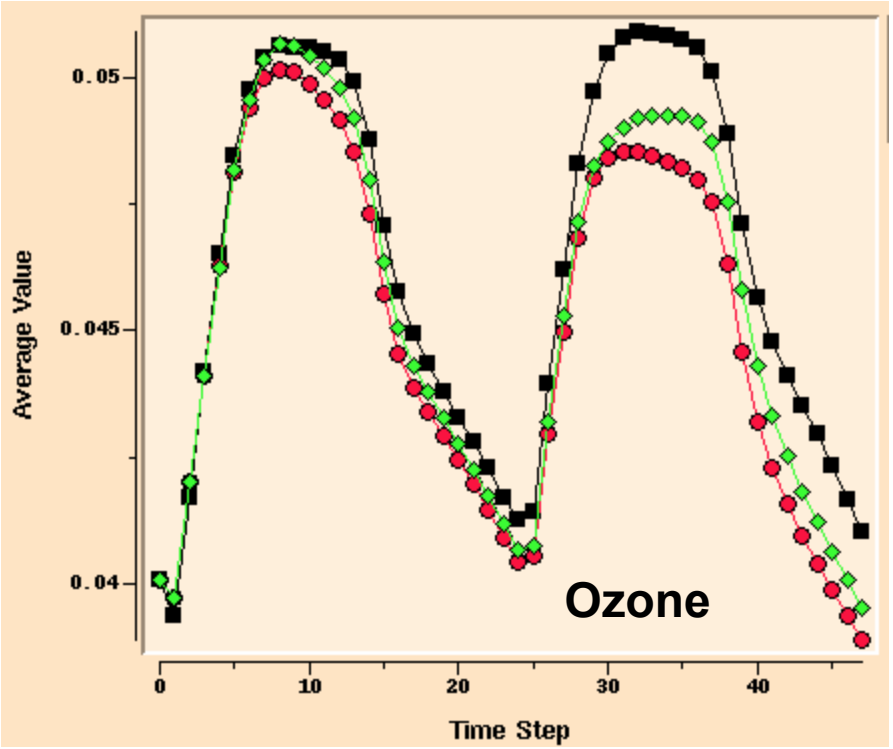
California Sub-domain average time series: July 18-19, 2006

Black (Loose), **Red** (Tight w/ISOP error), **Green** (Corrected Tight)



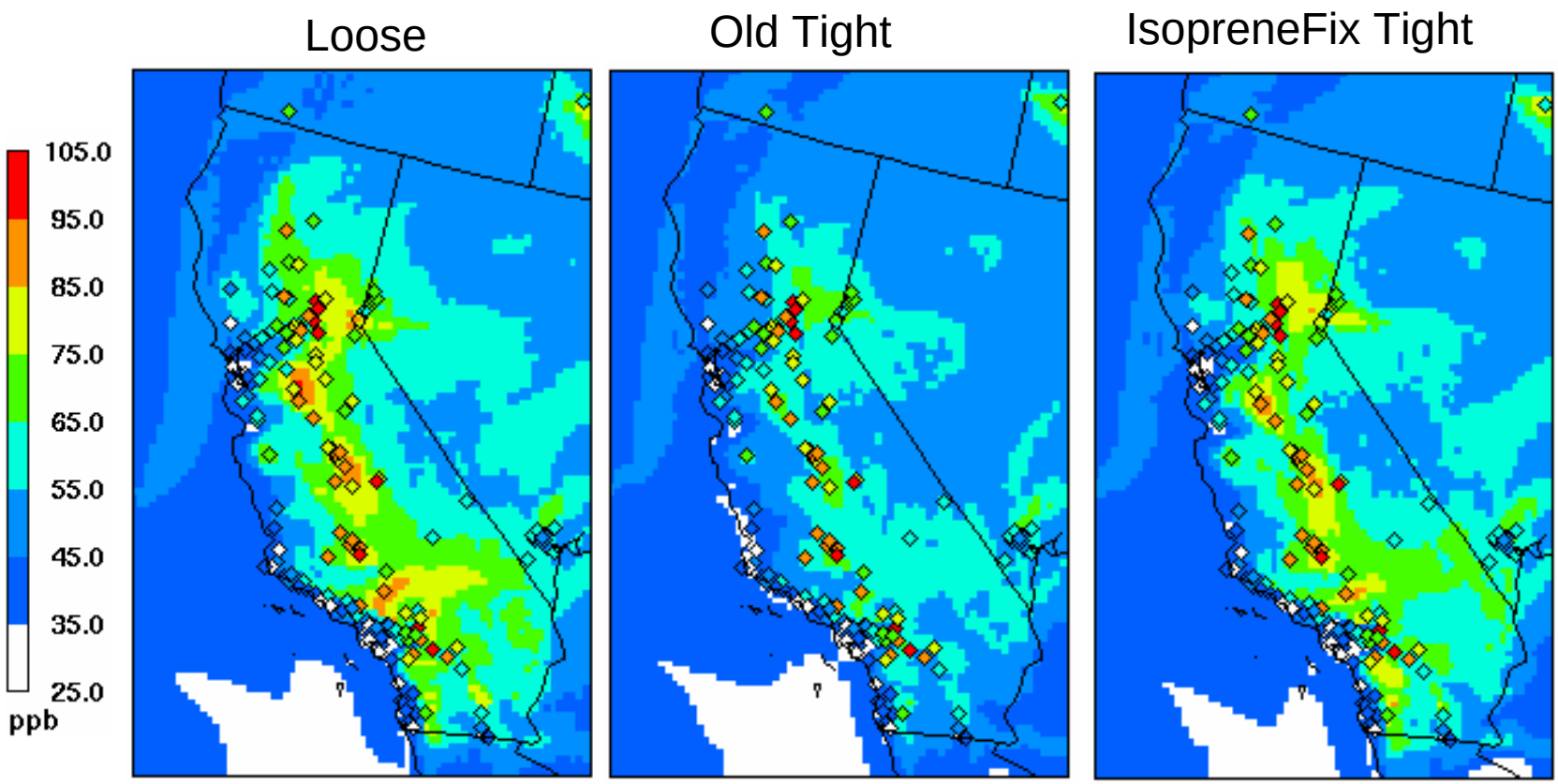
NTR: Inert organic nitrate in CBM-IV





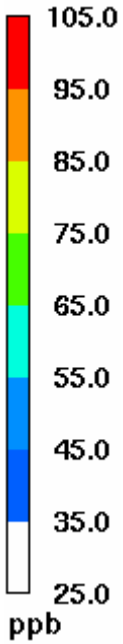
Correcting the low-bias in Experimental 5X Runs

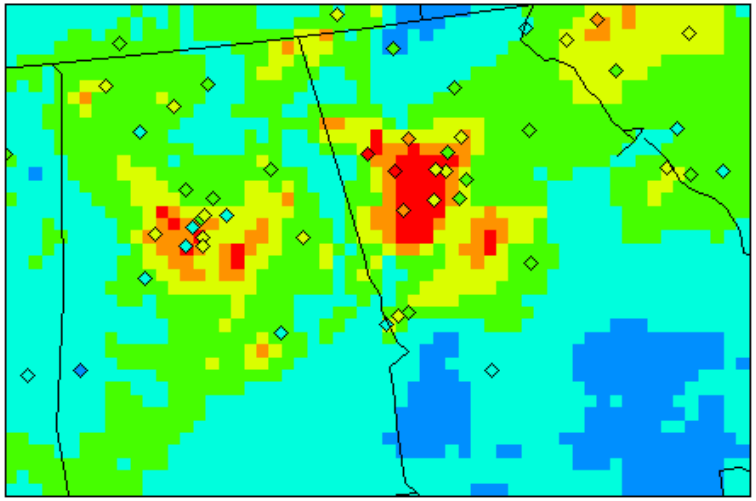
Max.-8hr O_3: 7/19/06



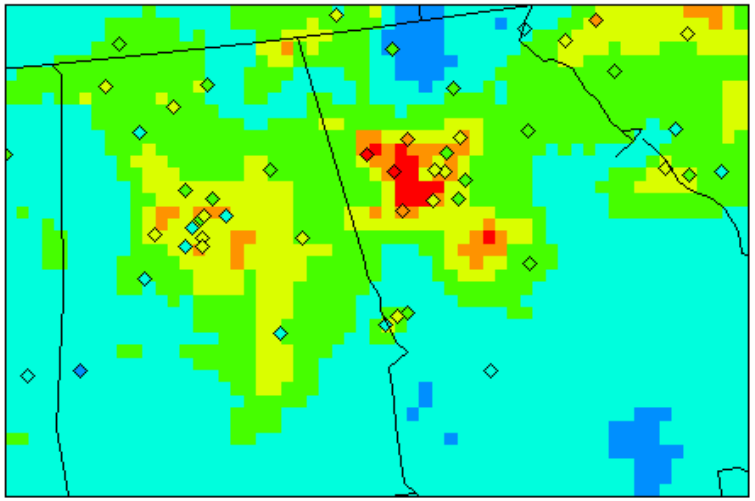
Correcting the low-bias in Experimental 5X Runs

Max. 8 O3
7/19/06

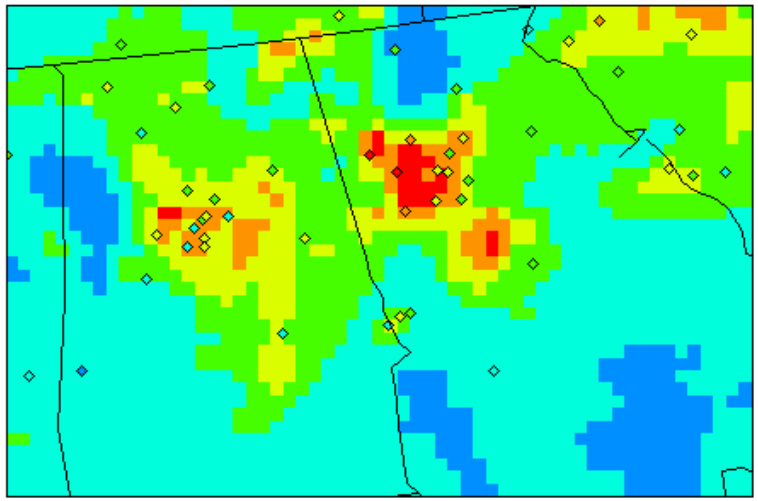




Loose



Old Tight

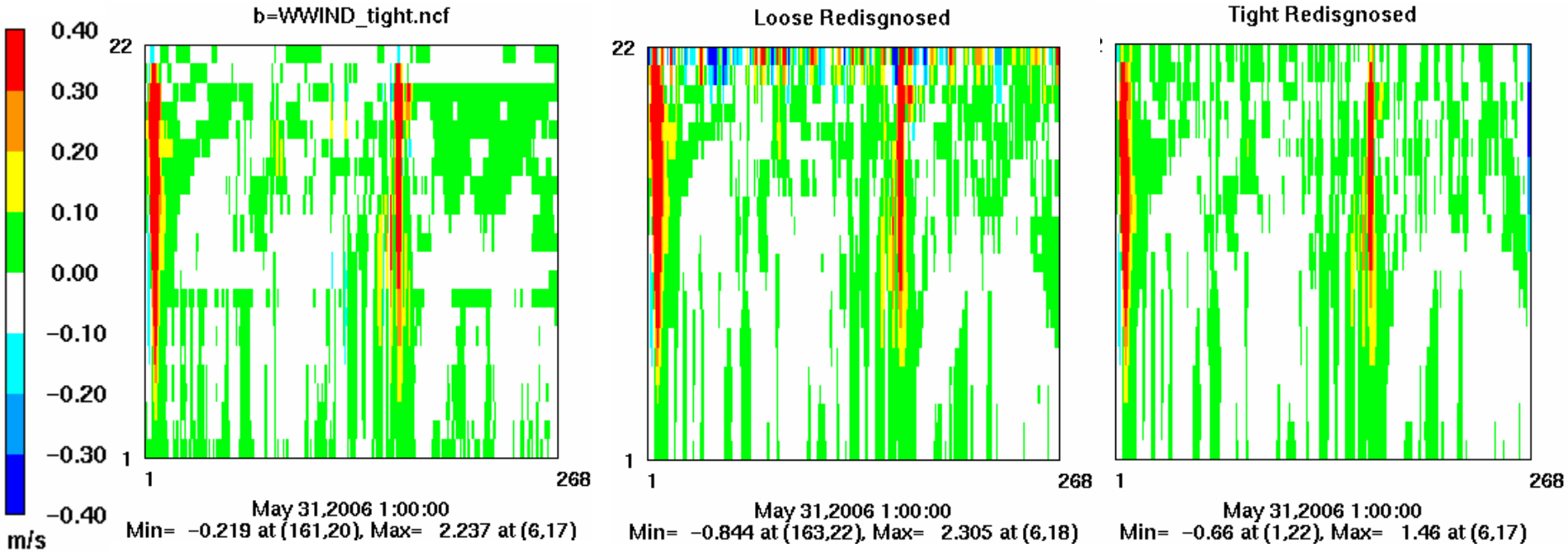


Isoprene Fix Tight

Improvements from Tight Coupling

Mass-consistent advection

Vertical Velocity Cross-sections



Tight coupling helps reproduce WRF-NMM vertical velocity fields with higher fidelity
Note: Large discrepancies at model top in loose-coupling

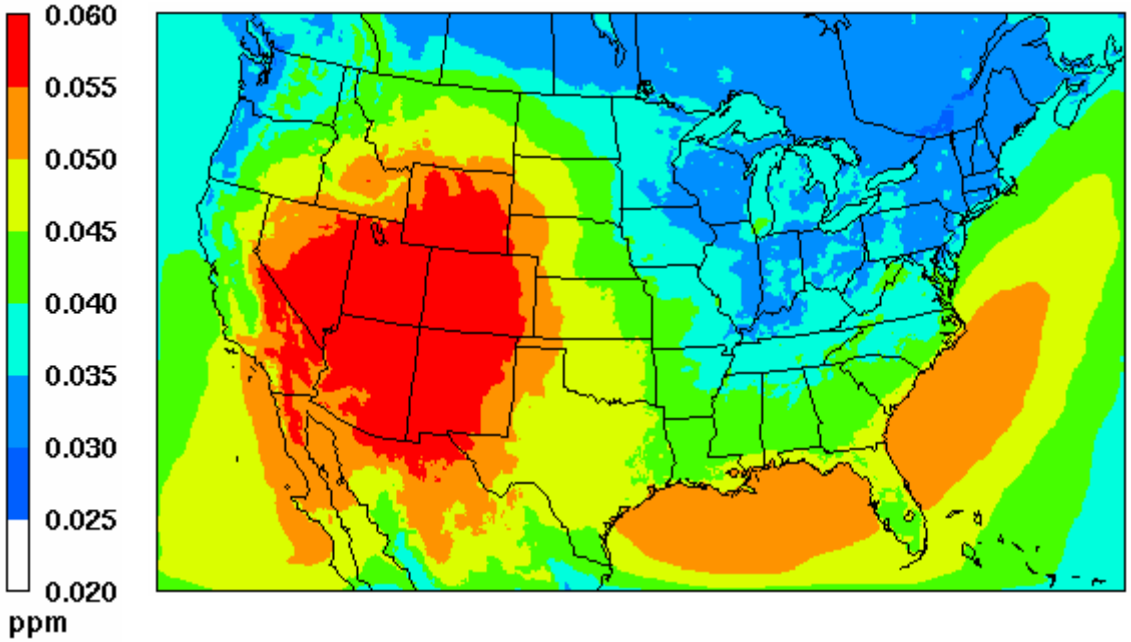
Lateral Boundary Condition Specification

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

- **Approach in Operational Runs**: Combination of
  - **Static default profiles**
    - "Clean" tropospheric background values
  - **Top most CMAQ-layer**: 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
- **Approach in Experimental Runs**
  - **Static default profiles**
  - **Added diagnostic tracers** to quantify "model background" O_3
    - Tracked impact of lateral boundary conditions (surface-3km and 3km-model top)

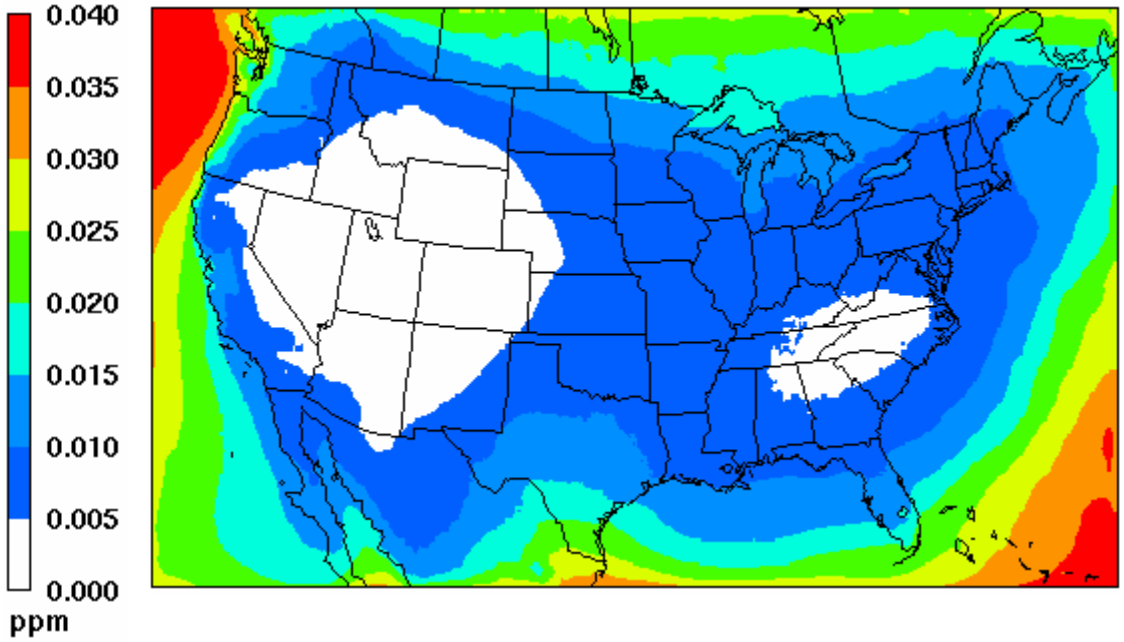
Modeled surface-level "background" O_3

Average from July 1-August 22, 2006

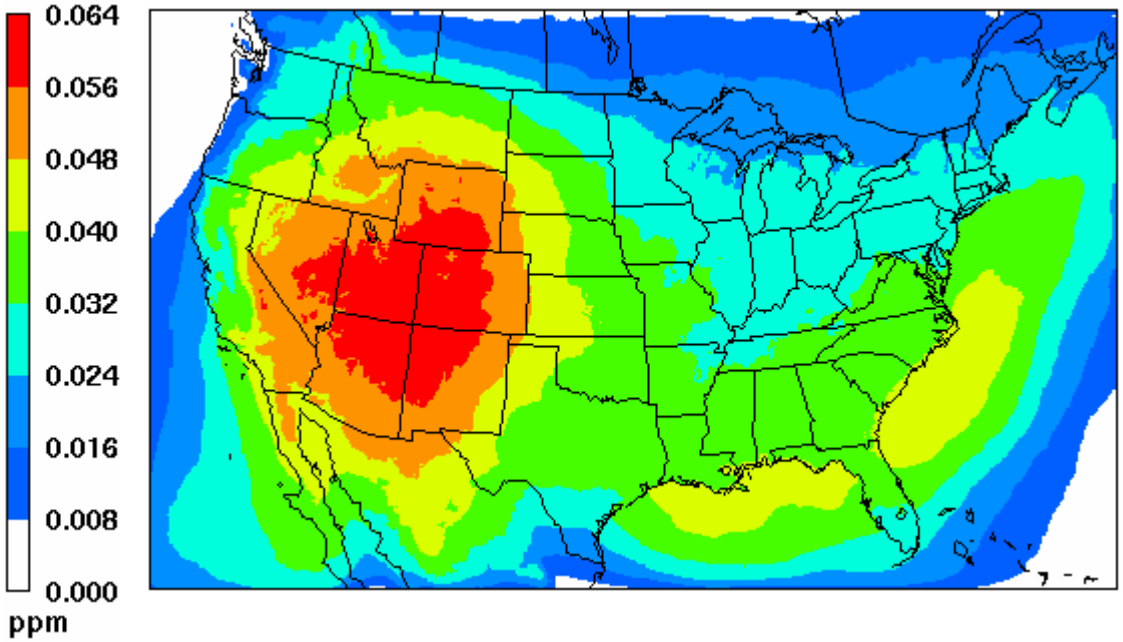


Background O_3 distributions are spatially heterogeneous

Components of modeled surface-level "background" O_3

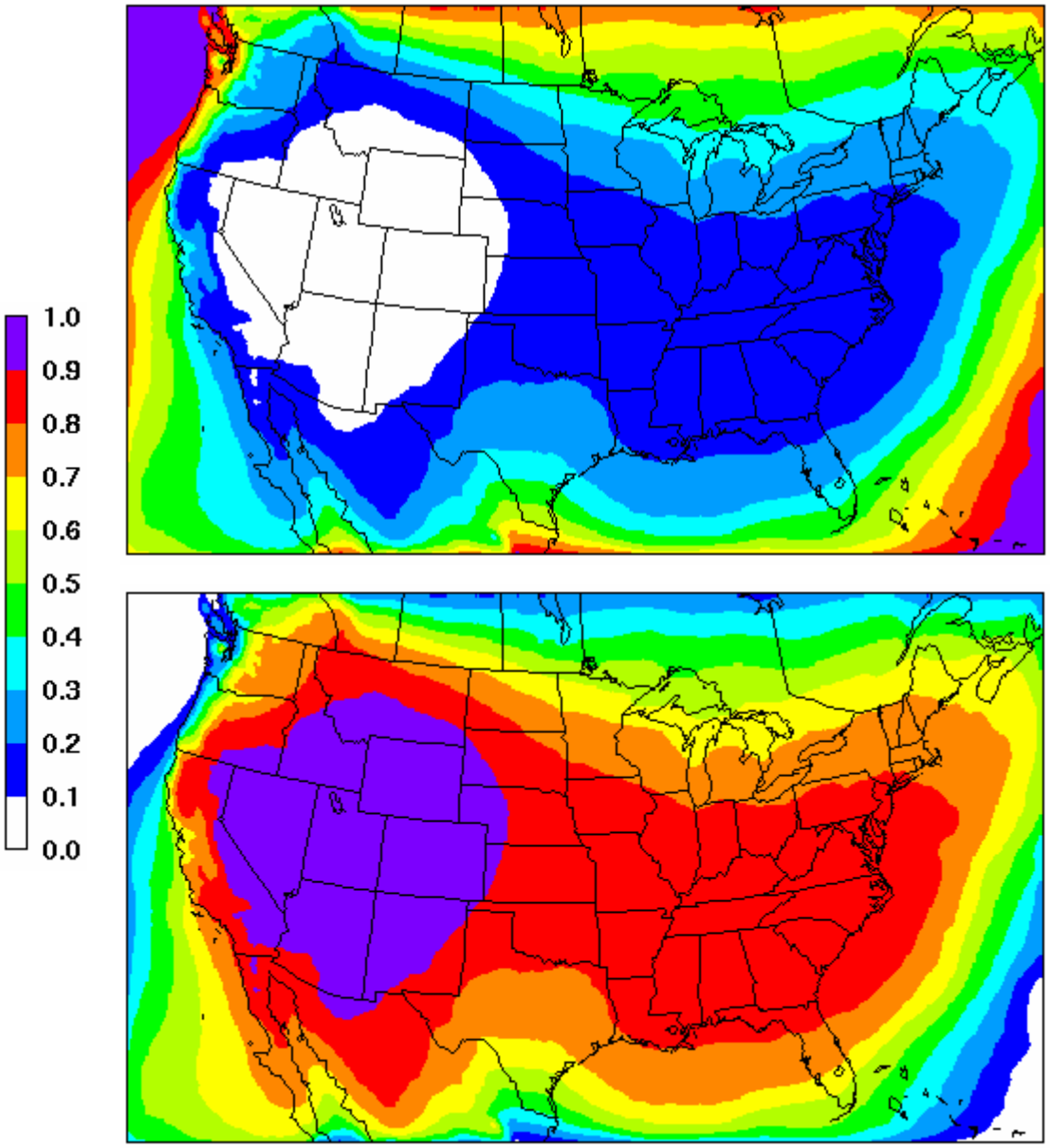


"Boundary Layer"
Surface – 3km



"Free Troposphere"
3km – Model top

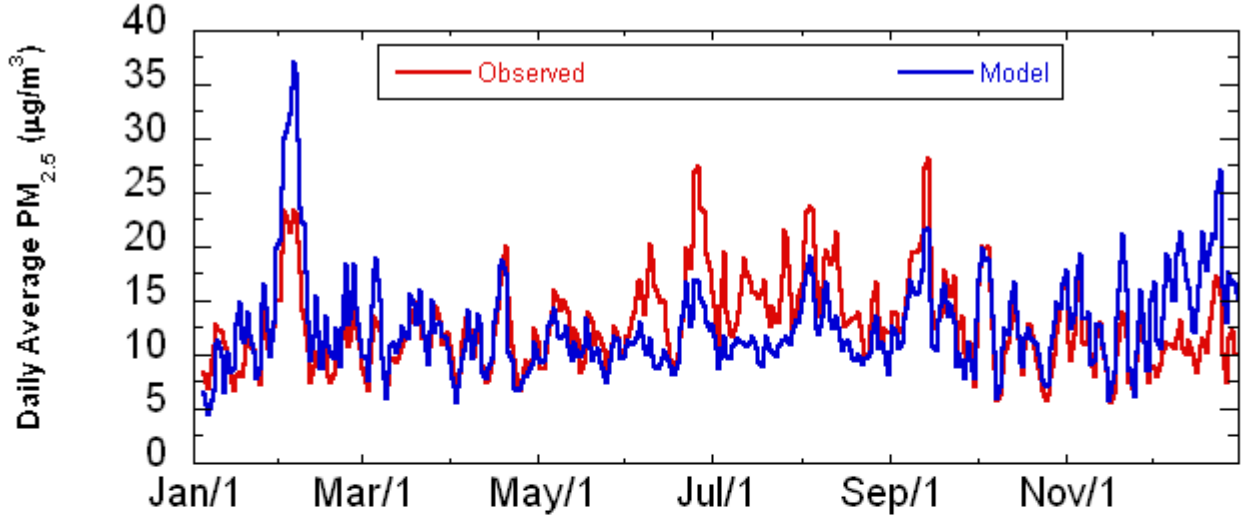
Components Modeled "background" O_3: Relative Contributions/Fraction



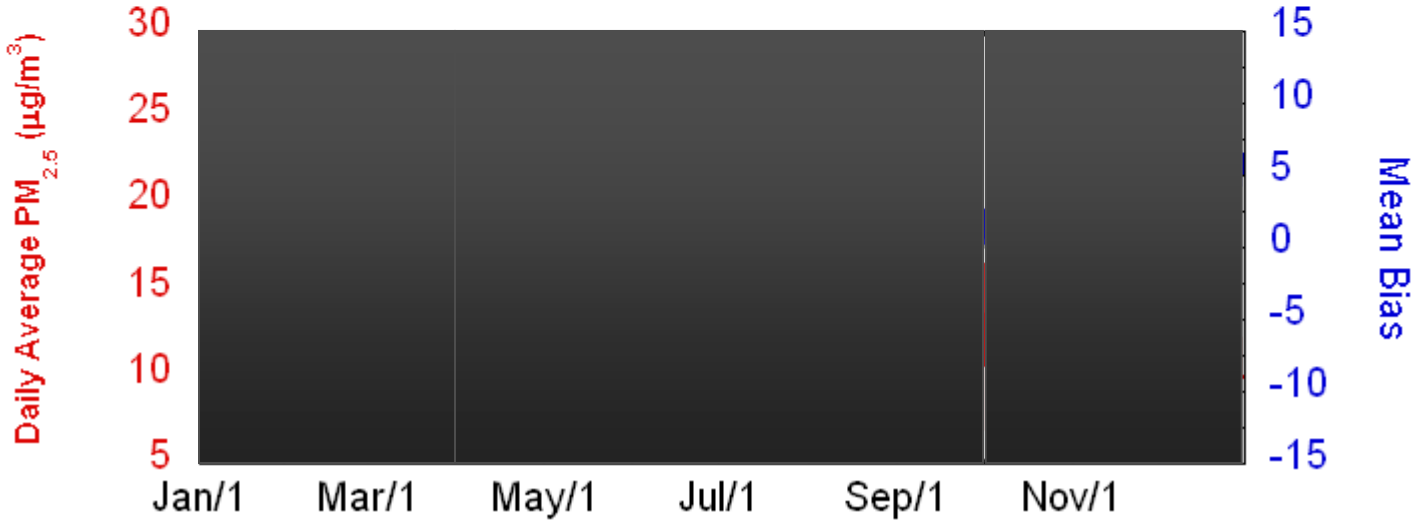
"Boundary Layer"
Surface – 3km

"Free Troposphere"
3km – Model top

Performance Summary for $PM_{2.5}$ over a year: 2005

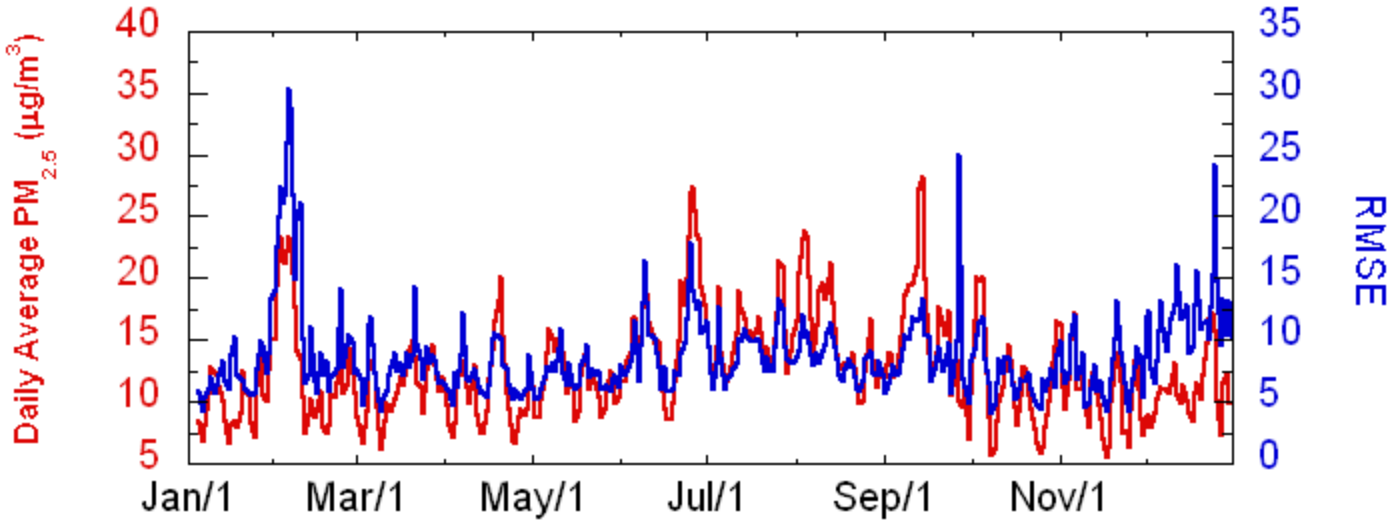


Captures day-to-day variability



Warm-season Under-prediction
Cool-season Over-prediction

Performance Summary over a year: 2005



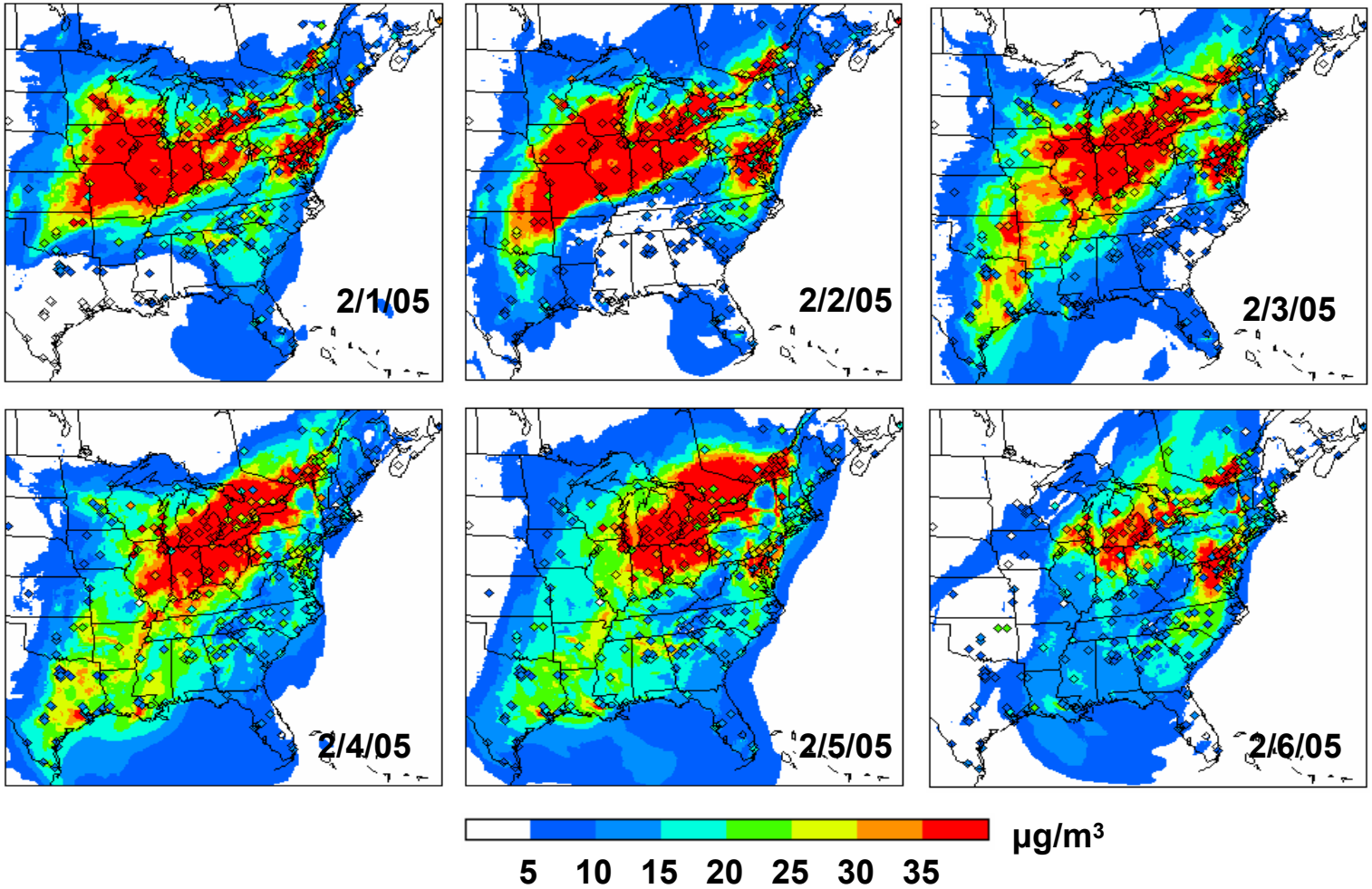
Larger errors at higher concentrations

Winter high bias

- Possible measurement bias
- Role of dynamics
- Unspeciated “Other” PM is biased high

Model Performance Characteristics: Winter 2005

Model and Observed Daily Average Surface $PM_{2.5}$

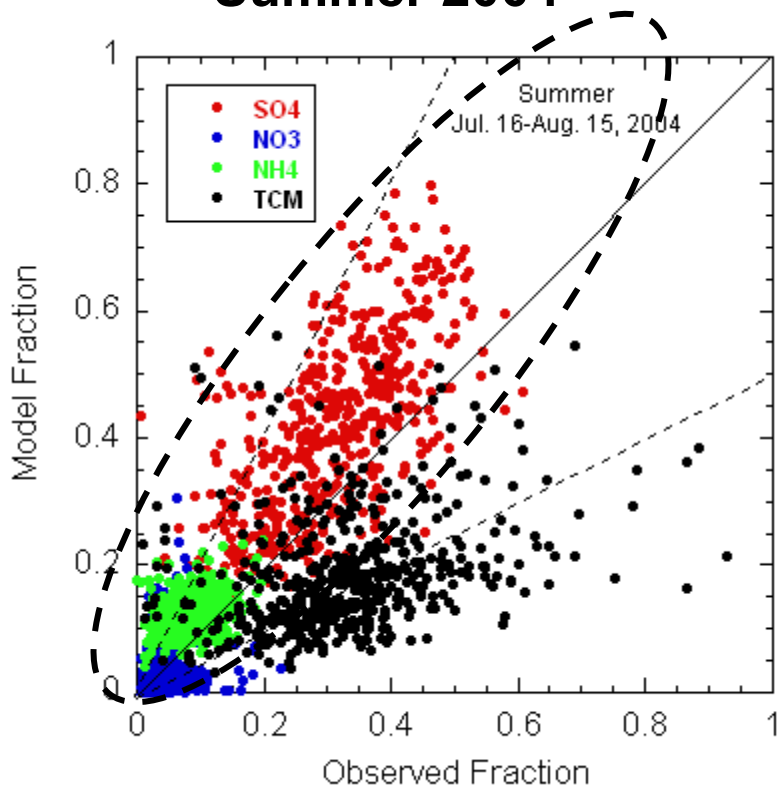


Capture hot-spots, tendency to over-predict

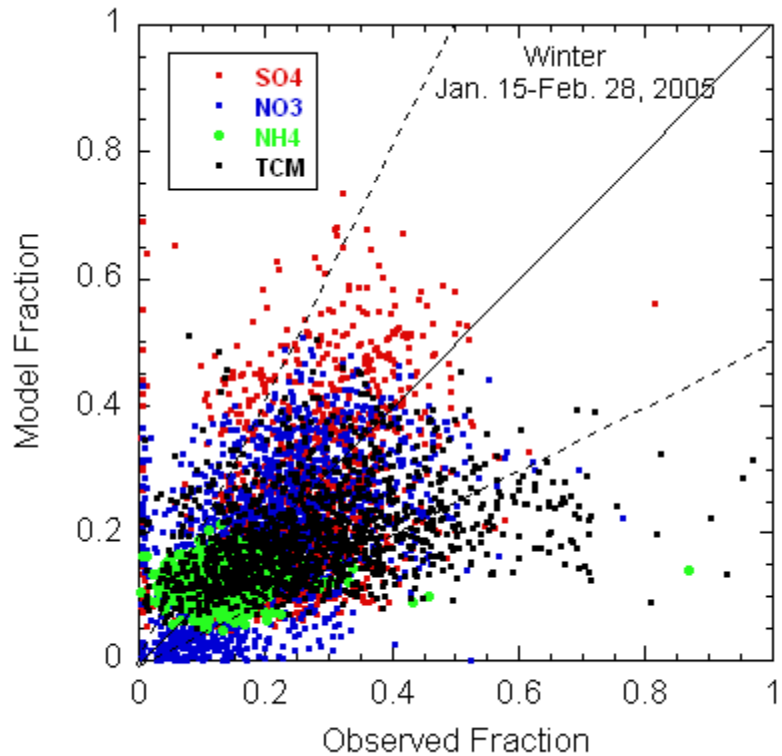
- ***possible role of mixing; K_{zmin} and/or PBL height ?***

$PM_{2.5}$ Compositional Characteristics
STN Measurements

Summer 2004



Winter 2005

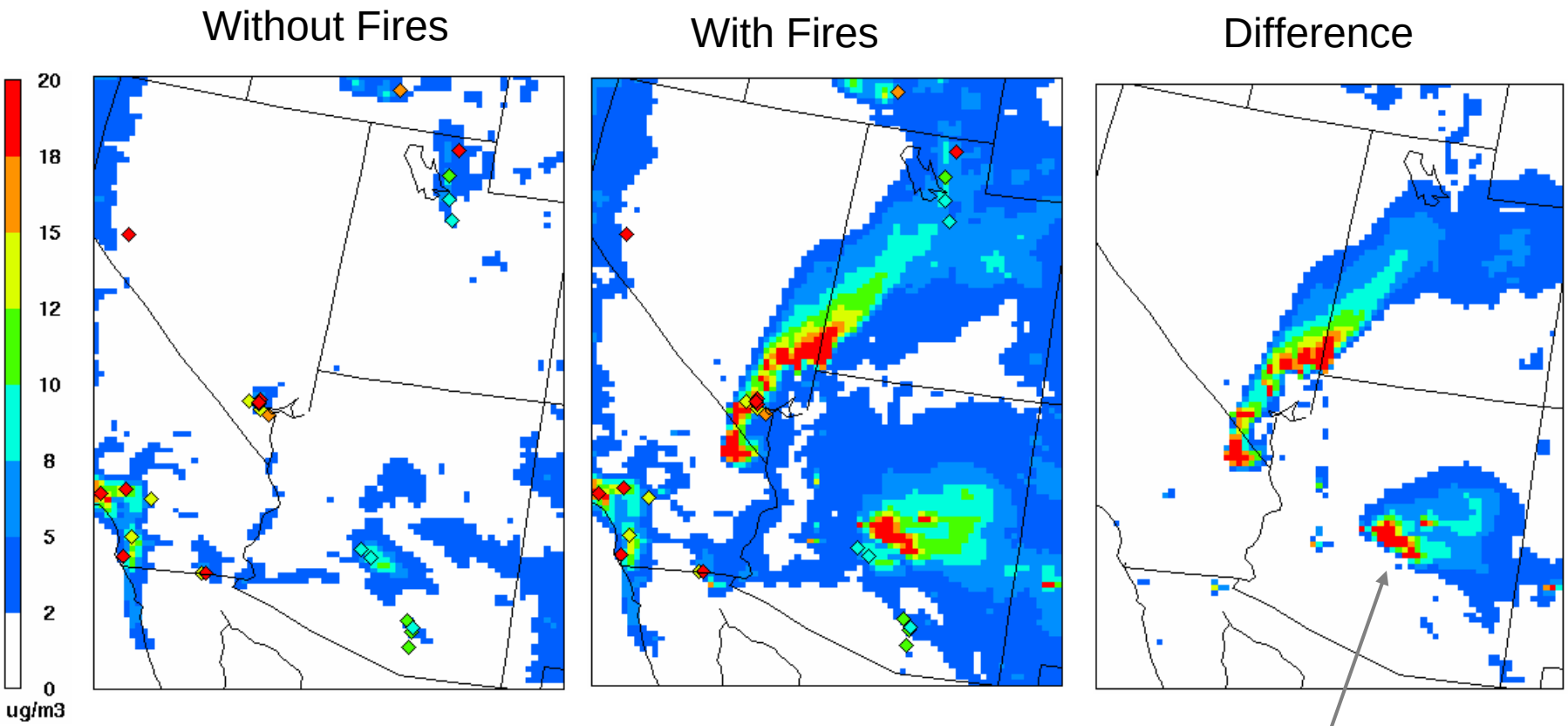


- Reasonable representation of Inorganic compositional characteristics
  - *Sulfate fraction over-predicted*
  - *Organic fraction under-predicted*

- Nitrate is a bigger player
- Larger OC fraction
  - under-predictions at lower concentrations

Specification of "Real Time" Emissions

Testing HMS-HYSPLIT fire emissions algorithm



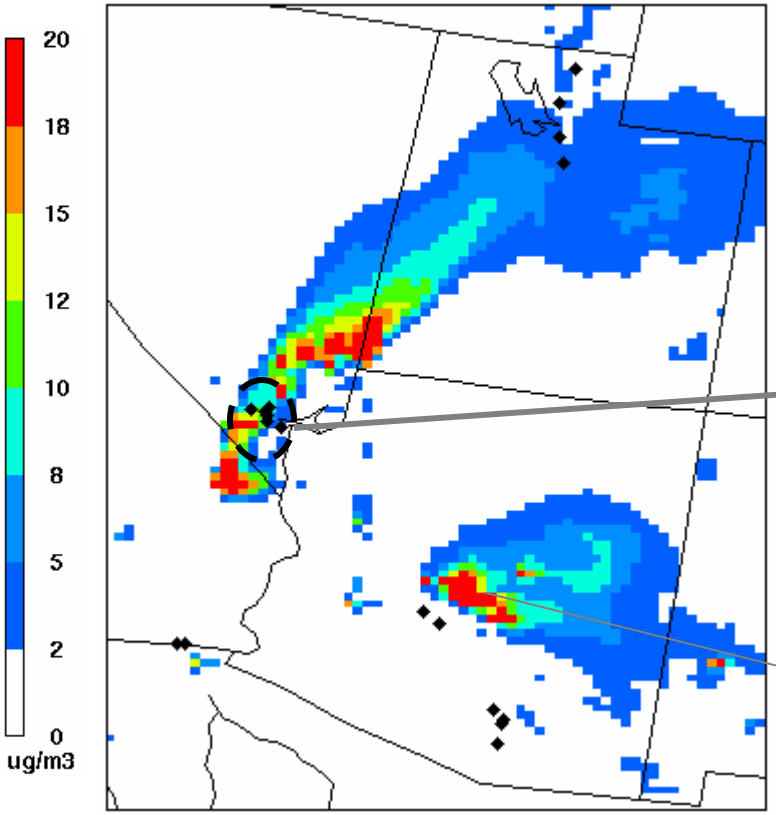
June 24, 2005: Daily Avg. $PM_{2.5}$

Cave Creek Complex fire began as two lightning-sparked fires on June 21, 2005. Became second largest fire in Arizona history.

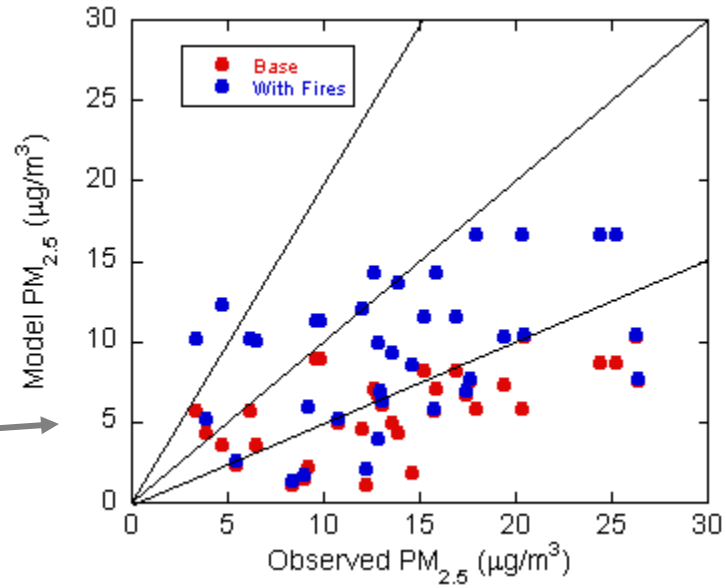
Specification of "Real Time" Emissions

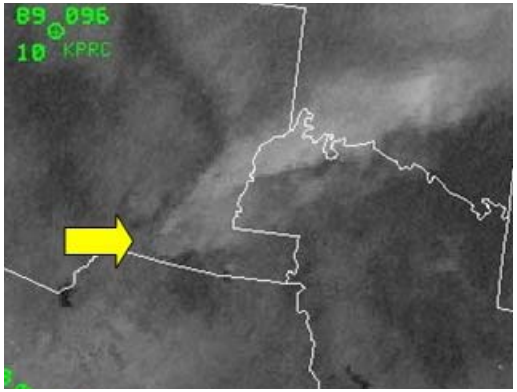
Testing HMS-HYSPLIT fire emissions algorithm

Fire plume signatures: June 24, 2005



June 21-26, 2005 Daily Avg.: Southern NV sites





June 24, 2005

Real-time specification of fire emissions improves PM forecast skill

Summary/Looking Ahead

- AQF system transitioned to WRF-NMM
  - Growing pains with a new and evolving modeling system
- WRF-NMM based dry-deposition velocities are higher than those derived from Eta
  - Persistent sink- can systematically impact predicted O_3
- Implemented the first step in tighter coupling between CMAQ and WRF-NMM computational grids
  - CMAQ calculations using the WRF-NMM vertical coordinate
  - Modifications to CMAQ to use the E-grid and rotated lat/lon coordinate underway
- Under-predictions for surface O_3 in experimental predictions were found to arise from error in isoprene emission calculations
  - Un-initialized lat/lon fields

Summary/Looking Ahead

- Initial analysis of boundary tracers indicate that *modeled O_3 background values are strongly influenced by free tropospheric LBC* values
  - Locations at which O_3 is over-predicted generally also correspond to high background but low observed values
- Rigorous analysis of developmental PM simulations underway
  - Seasonal trends/biases similar to hind-cast CMAQ applications
  - Speciated PM verifications with surface network (STN, CASTNet, IMPROVE, SEARCH) and aloft (ICARTT) data
- Conducted initial testing of a methodology for specifying "real-time" fire emissions
  - Initial results are encouraging