THE COMMUNITY MULTISCALE AIR QUALITY (CMAQ) MODEL:

Model Configuration and Enhancements for 2007 Air Quality Forecasting

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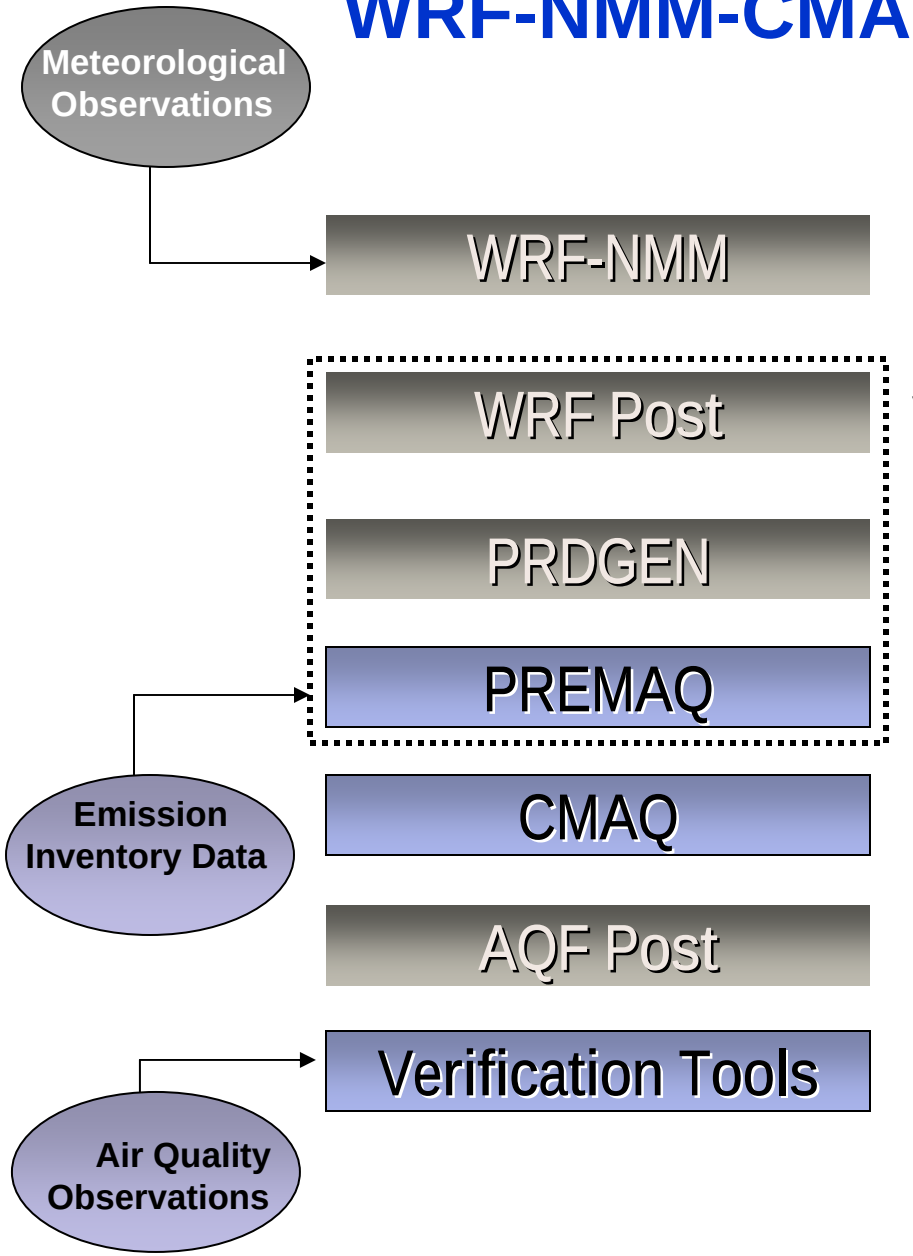
WRF-NMM-CMAQ AQF Capability



NAM Meteorology model

Vertical interpolation

Horizontal interpolation to Lambert grid

CMAQ-ready meteorology and emissions

Chemistry/Transport/Deposition model

Gridded product files for users

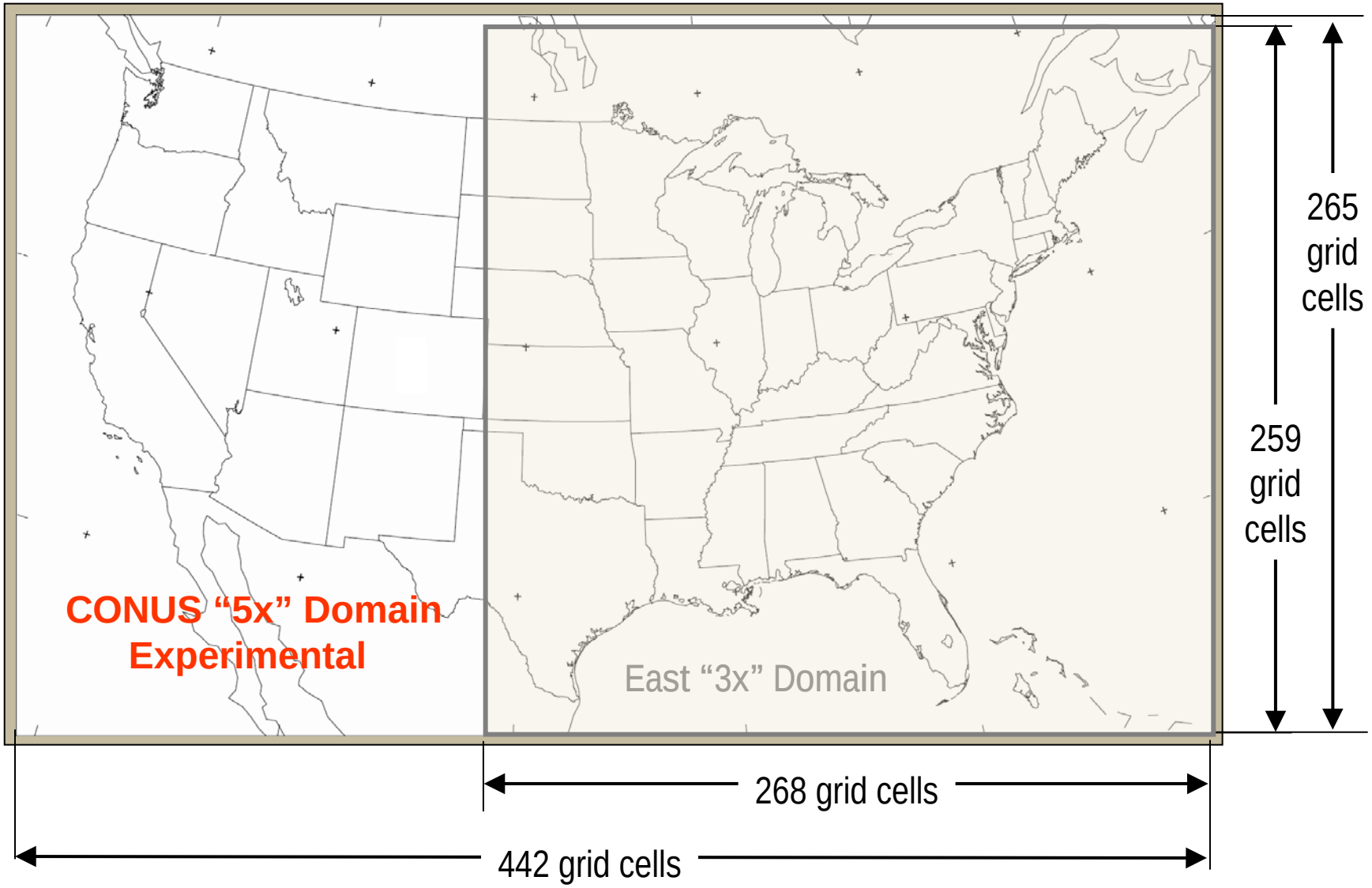
Performance feedback for users/developers

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
  - ***California non-road*** based on 2002 NEI
- 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
    - *Emissions also created using 2007 VMT and fleet projections but not incorporated due to under-predictions noted early in season; 7% reduction consistent with estimates from EPA OTAQ*
- 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

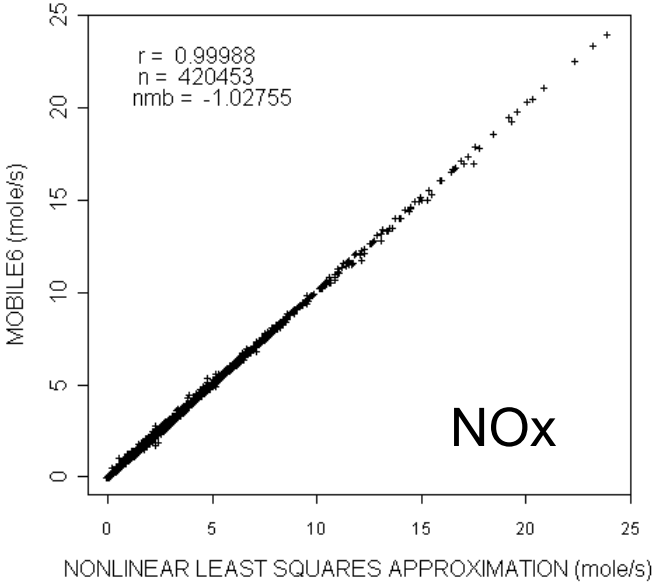
- Regression applied at each grid cell at each hour of the week for each species to create temperature-emission relationship

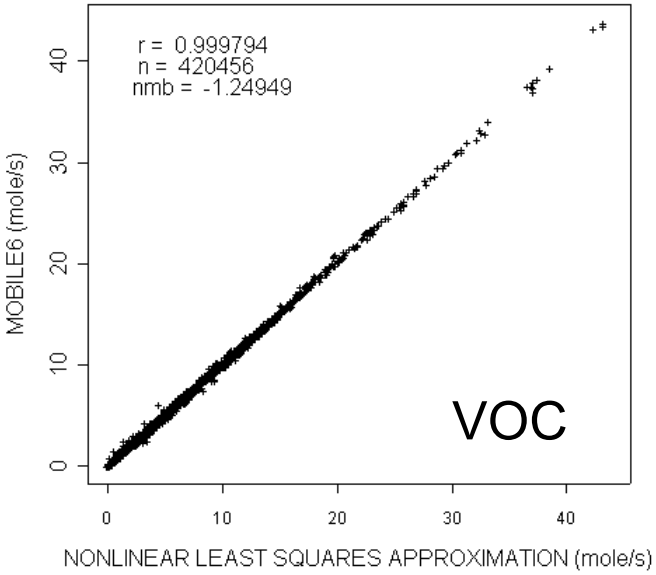
- Mobile Source emissions calculated in real-time using this derived temperature/emission relationship

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

- For California used 2001 mobile estimates from CARB

Monday

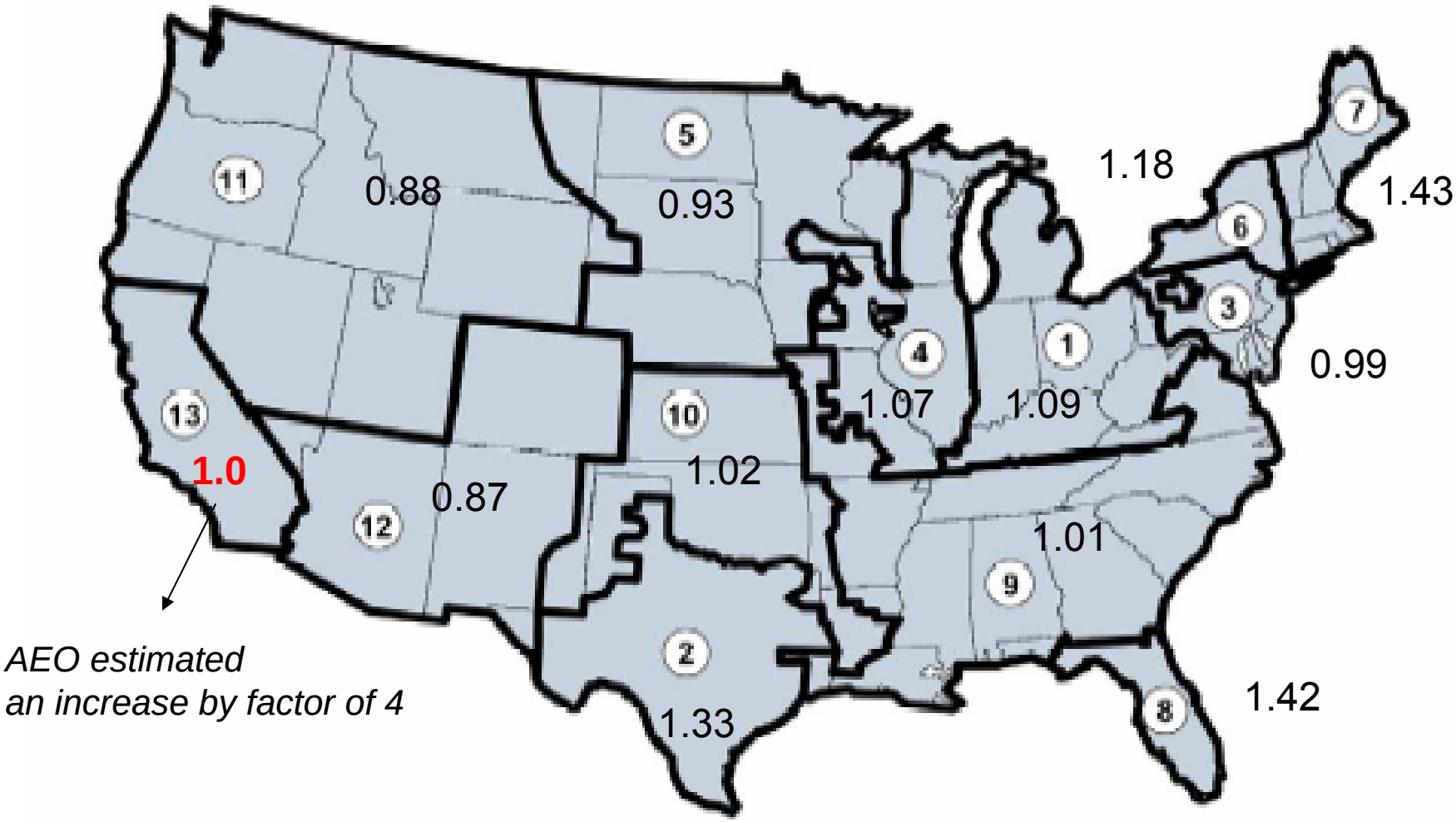




Point Sources

- 2005 Continuous Emissions Monitoring for NO_x and SO_2
  - Monthly temporal profiles on a state-by-state basis derived from CEM
- Modified EGU NOx emissions using DOE's Annual Energy Outlook (Jan. 2006)
  - Calculated 2007/2005 NO_x and SO_2 annual emission ratios on a regional basis (from DOE data)
  - *Exception California*
- For other pollutants and non-EGU: 2001 NEIv3
  - Georgia non-EGU based on 2002 inventory from GADNR

EGU NO_X adjustments 2007/2005 by region



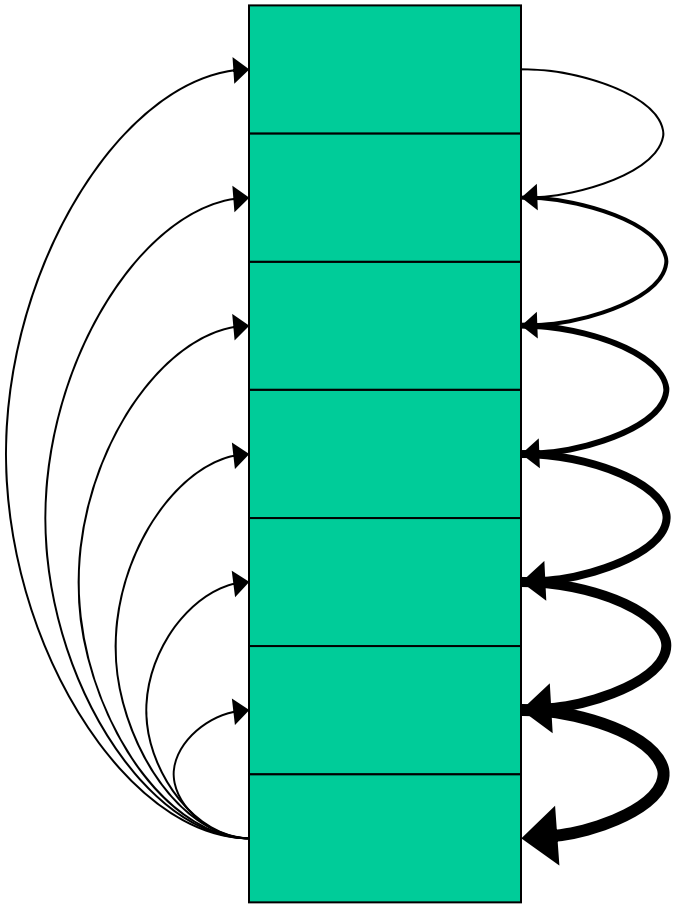
Source: derived from Department of Energy Annual Energy Outlook 2007 http://www.eia.doe.gov/oiaf/aeo/index.html

CMAQ Configuration

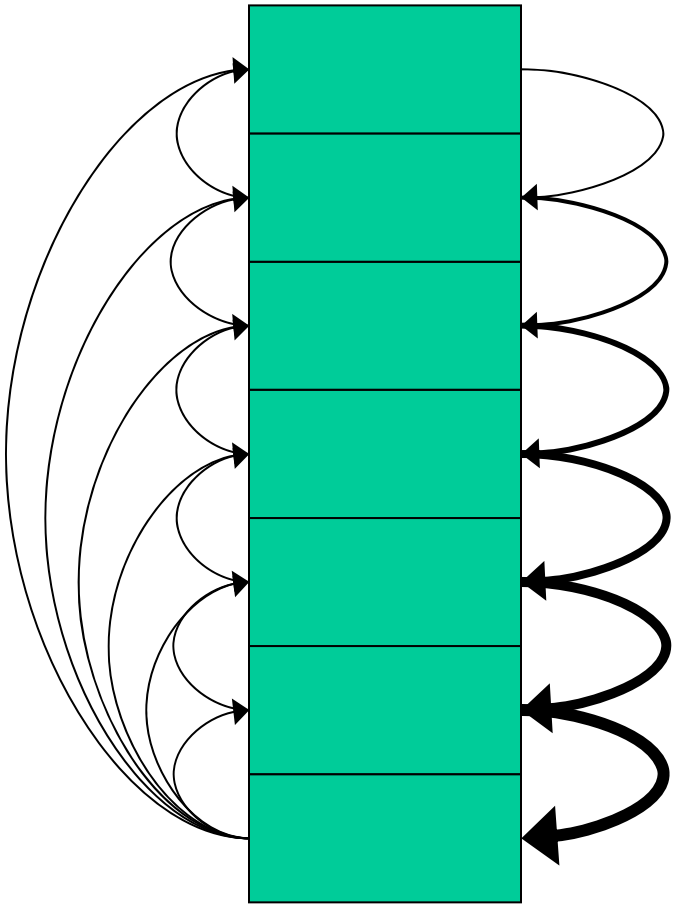
- **Advection**
  - Horizontal: *Piecewise Parabolic Method*
  - Vertical: *Upstream with rediagnosed vertical velocity to satisfy mass conservation*
- **Turbulent Mixing** *(in operational 3x)*
  - K-theory; PBL height from WRF-NMM
  - Minimum value of K_z allowed to vary spatially depending on urban 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

Turbulent mixing in Experimental (5X)

J. Pleim, J. Appl. Meteor. Climat., 46(9), September 2007



ACM



ACM2

- Combination of local+non-local closure
- Includes effects of large convective eddies & small shear driven eddies

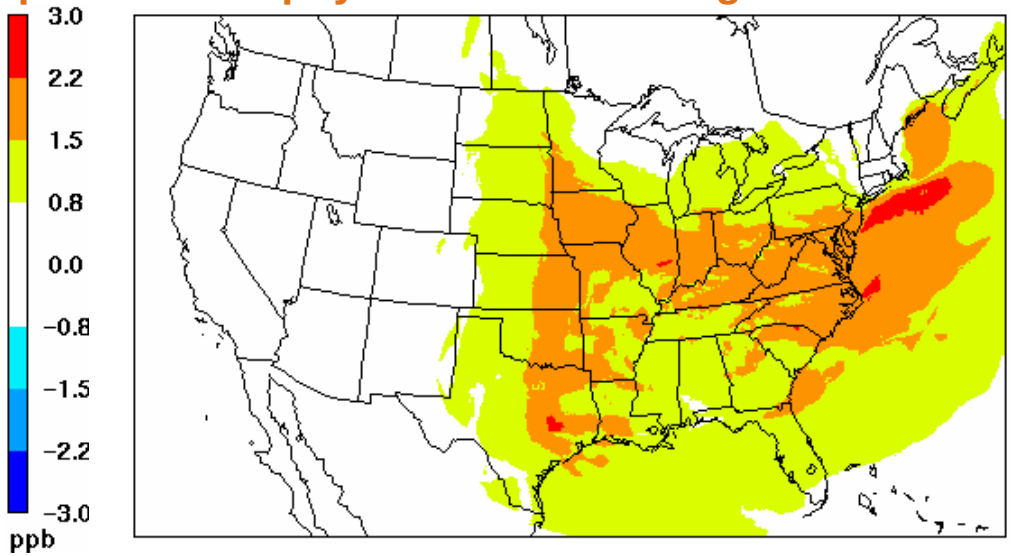
CMAQ Configuration (contd.)

- **Gas phase chemistry**
  - *CB4 mechanism with EBI solver*
    - ***Testing with CB05 initiated***
  - 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, *Atmos. Env.*)
    - **Used in Continental U.S. (5x) domain**

CMAQ Configuration (contd.)

- **Dry Deposition**
  - **Persistent sink for O3 – can impact predicted O_3**
  - Dry : M3dry modified to use WRF land surface parameters
  - Add mesophyll resistance for NO, NO_2 and CO
    - Decrease V_d for these species
    - ***Impact***: lower V_d for NOx, more NOx, generally more O_3, in some cases more titration
    - Impacts all operational, experimental, and developmental runs
  - Changes in WRF-LSM in June 2007 also impact V_{dO3}

Impact of mesophyll resistance change on max. 8-hr. O_3

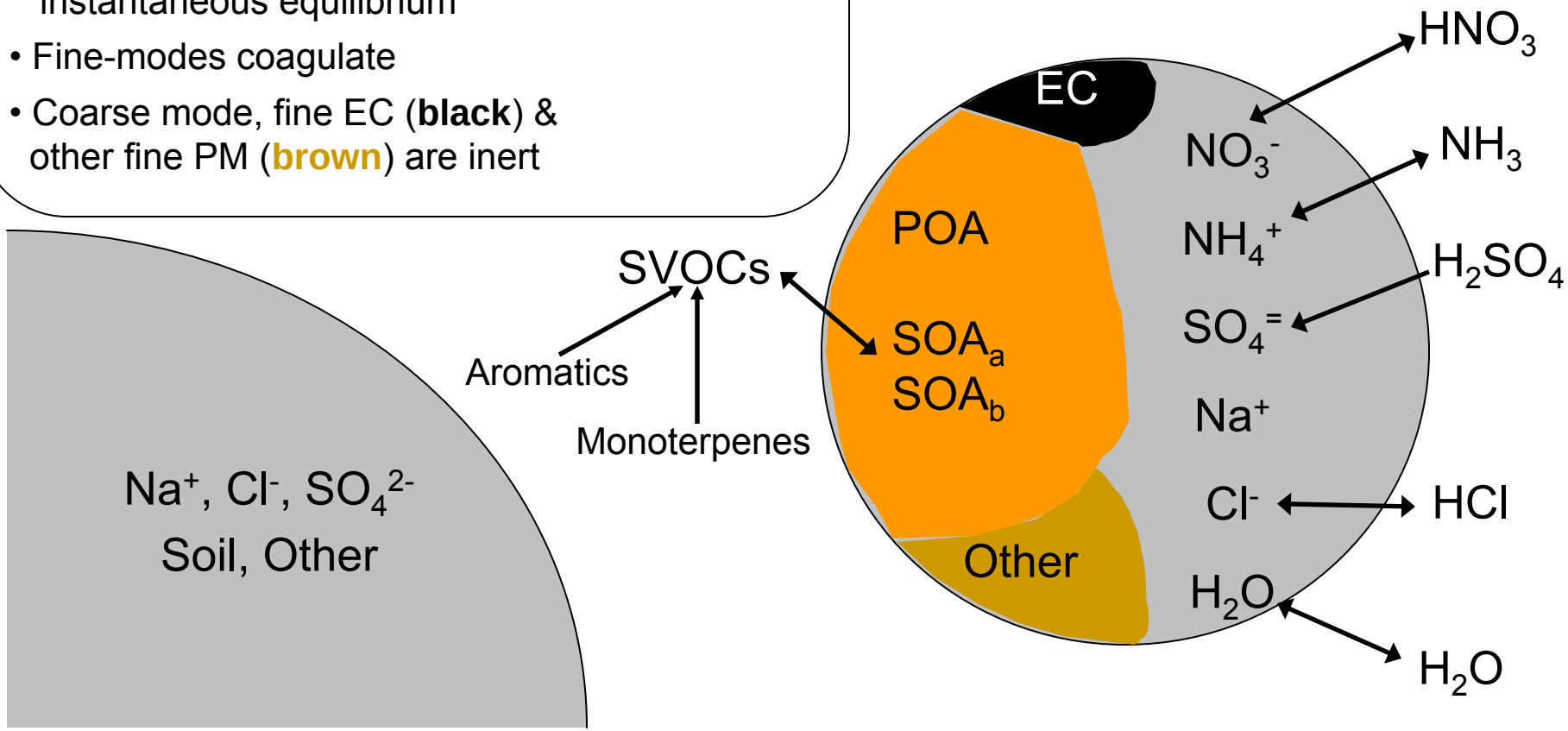


May 20, 2007

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

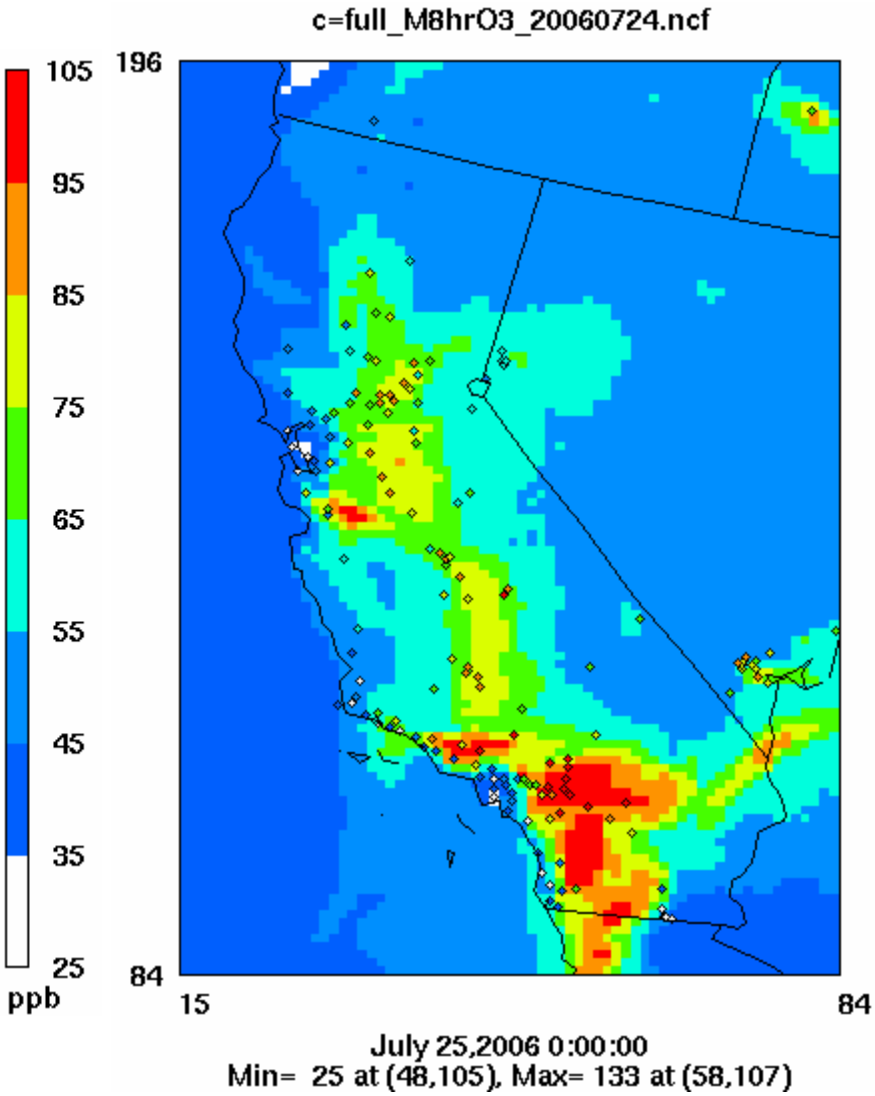


COARSE MODE

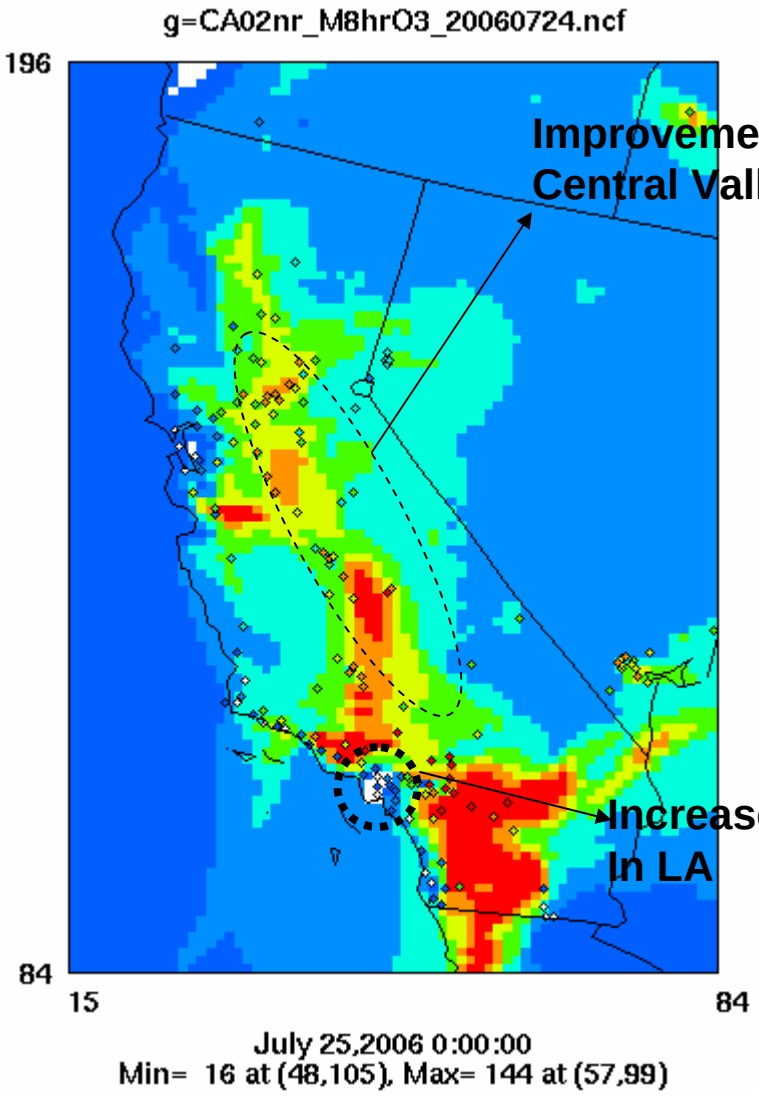
2 FINE MODES

CA emission perturbation sensitivity

BASE

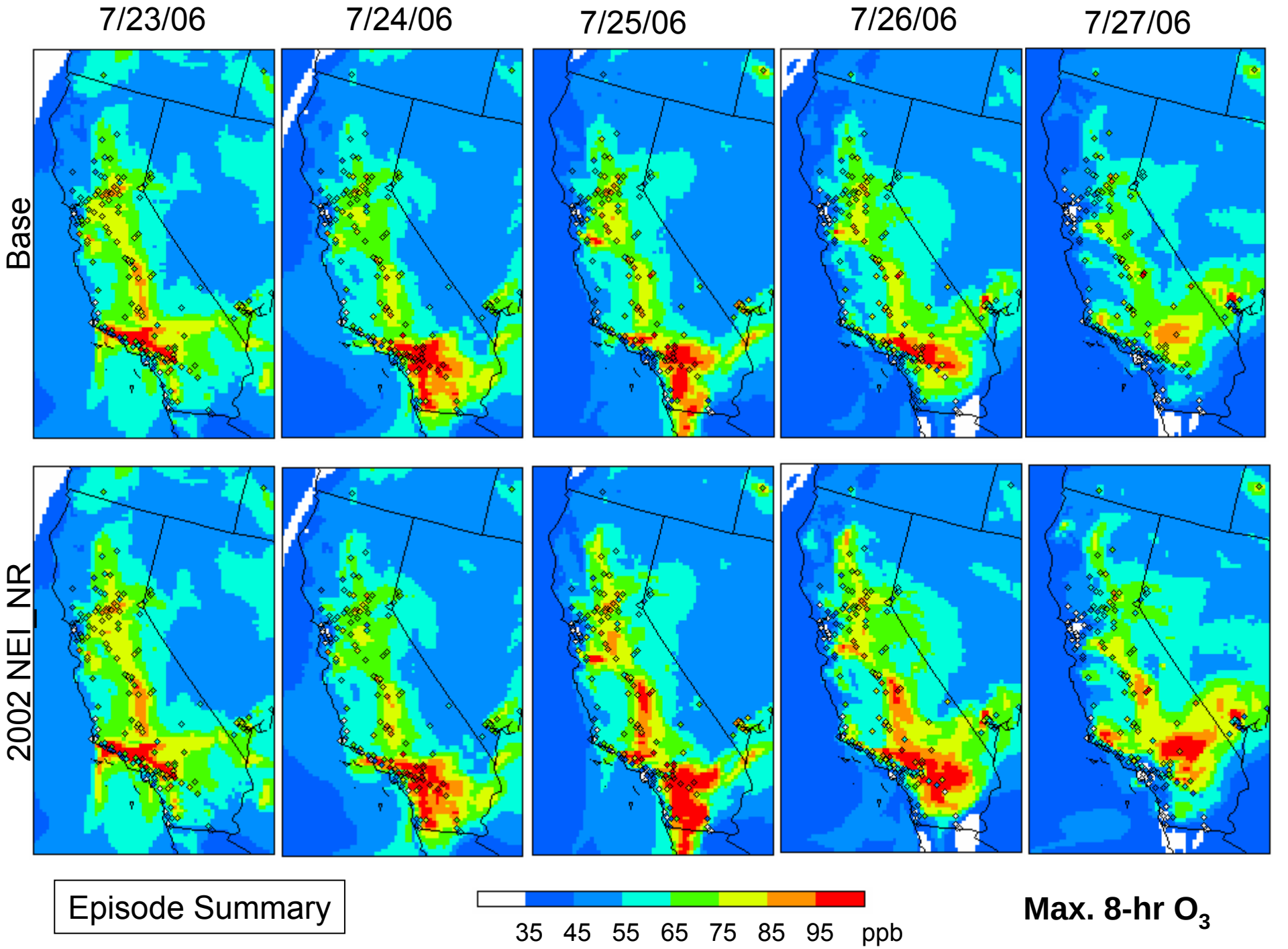


2002 NEI_NR



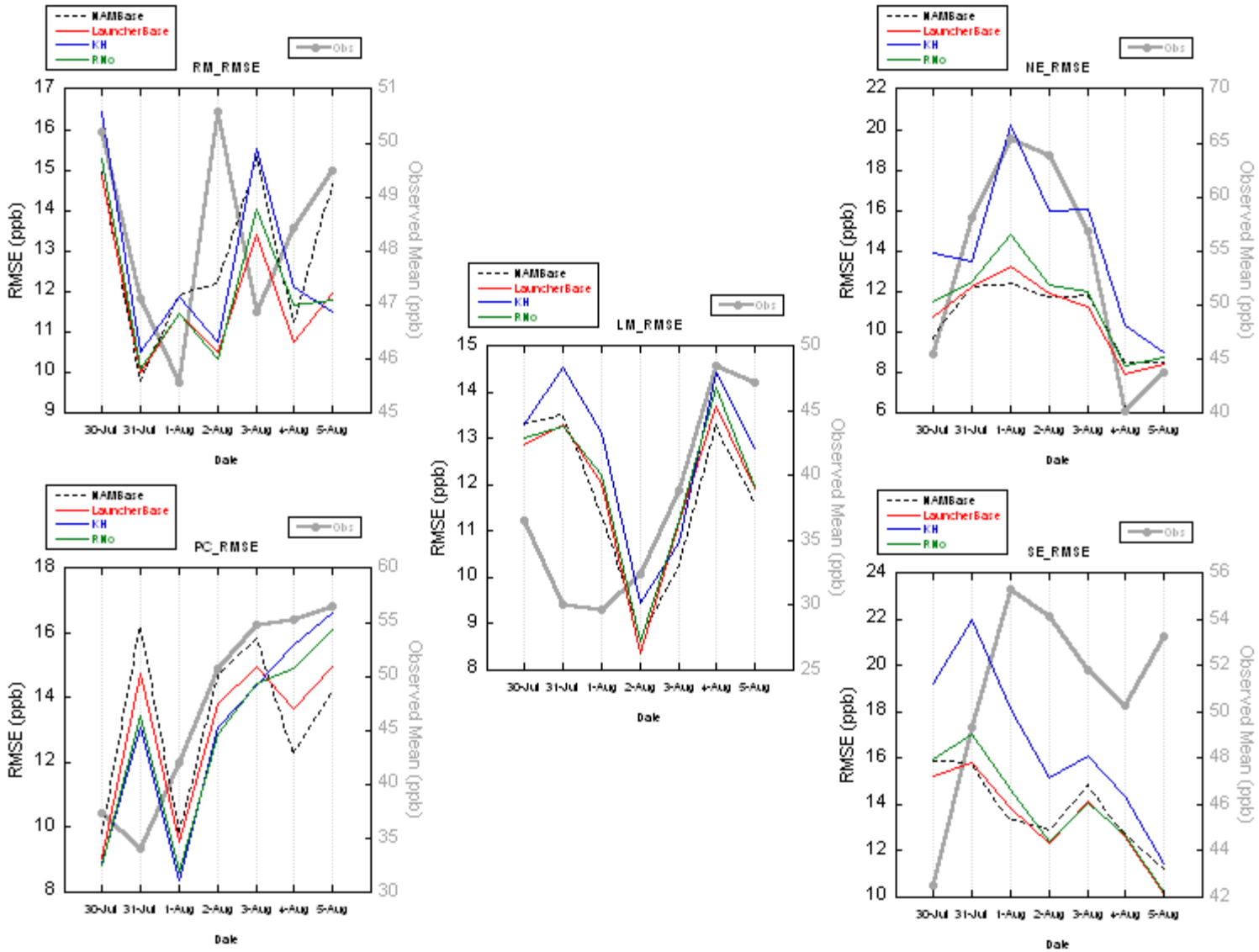
Improvements in Central Valley

Increased titration In LA


7/23/06
7/24/06
7/25/06
7/26/06
7/27/06
Base
2002 NEI_NR
Episode Summary
35 45 55 65 75 85 95 ppb
Max. 8-hr O_3

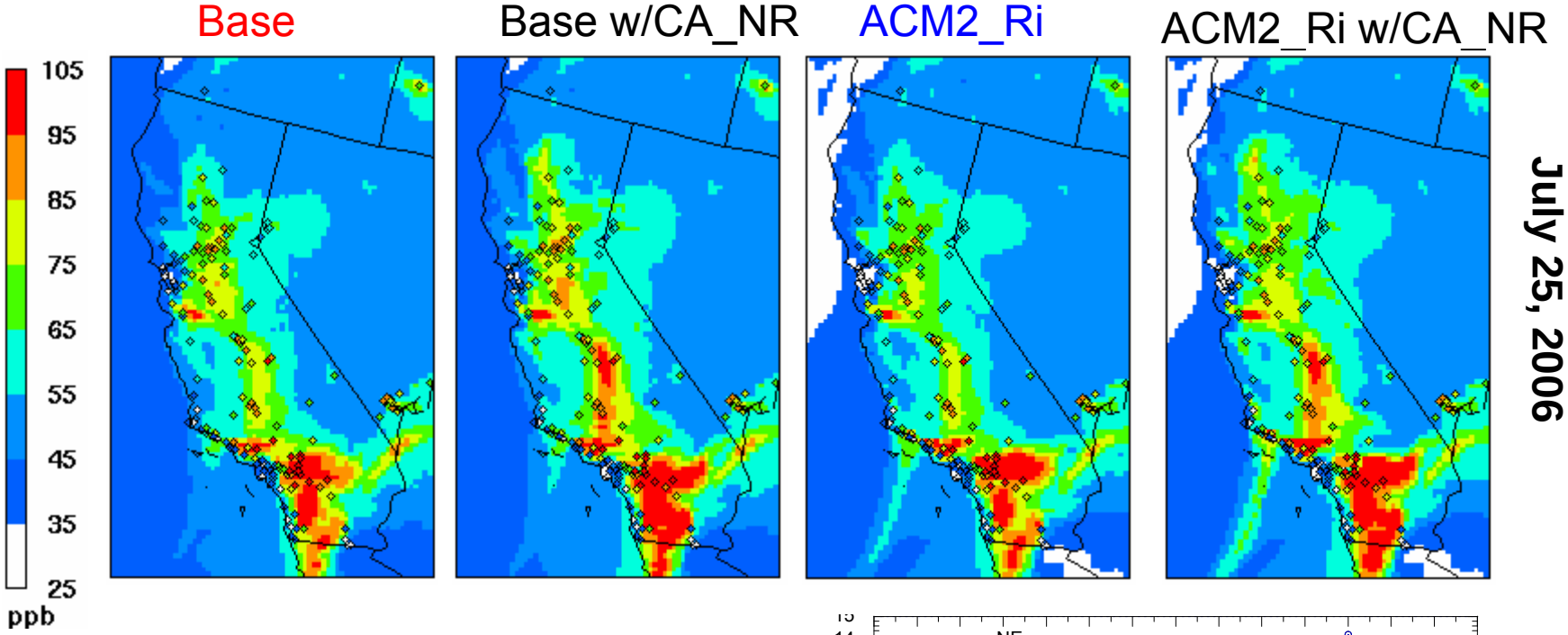
Retrospective Analysis: PBL Mixing Schemes

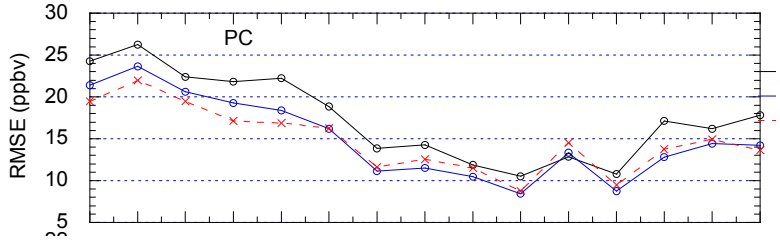
- - - - NAMbase — Launcherbase — KH — Rno

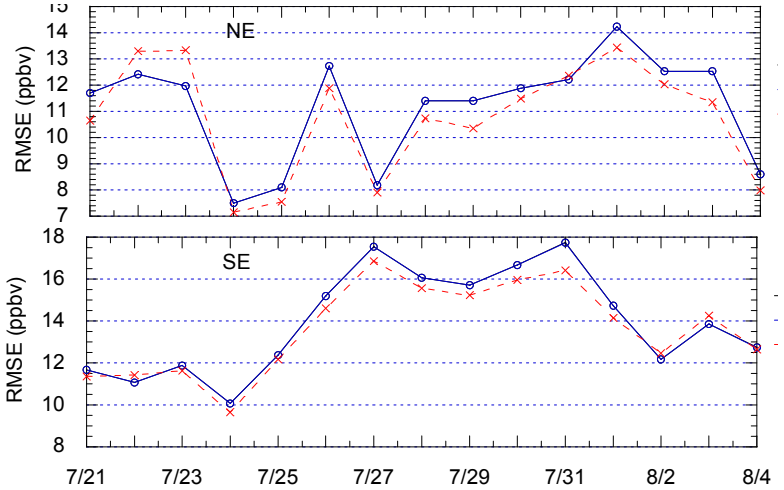


K_h from NAM: reduced low bias in CA, but resulted in high bias/error elsewhere

Retrospective Analysis: Combined PBL and Emissions Sensitivity

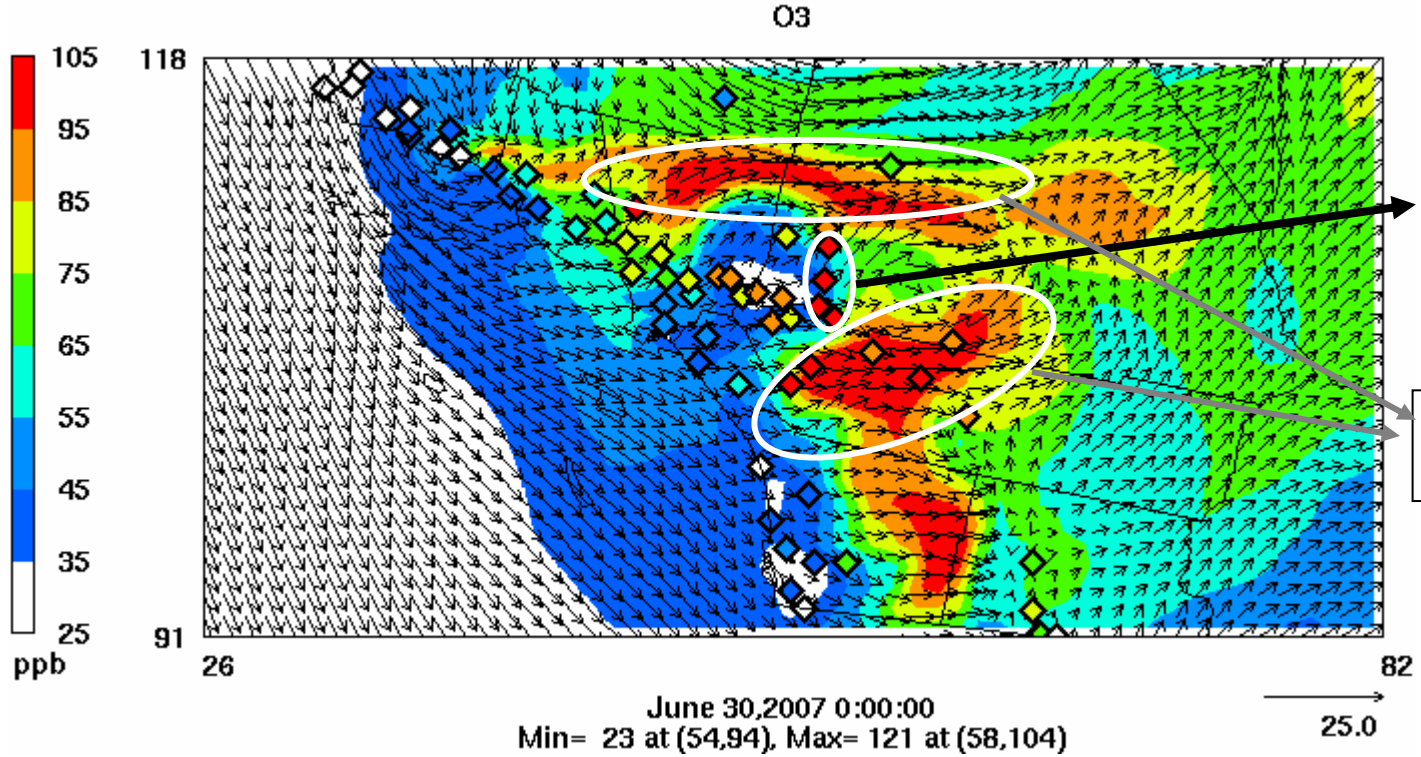






Slight increase in O_3 and RMSE with ACM2

Under-predictions in LA Basin

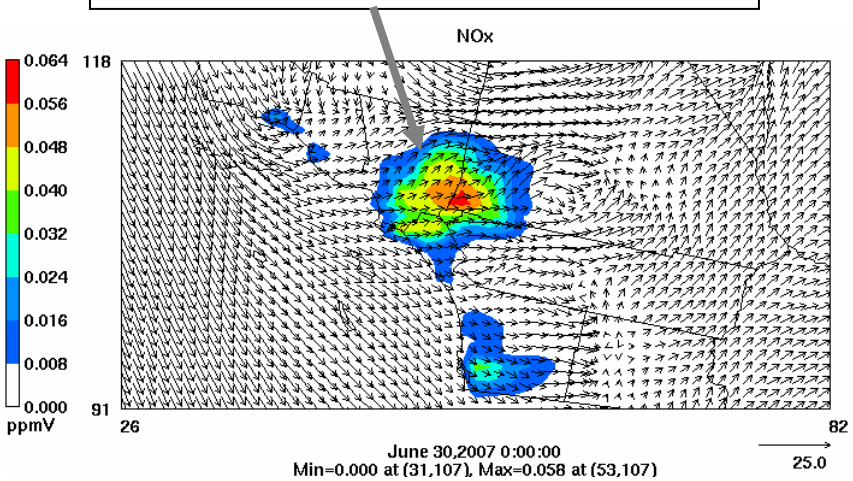


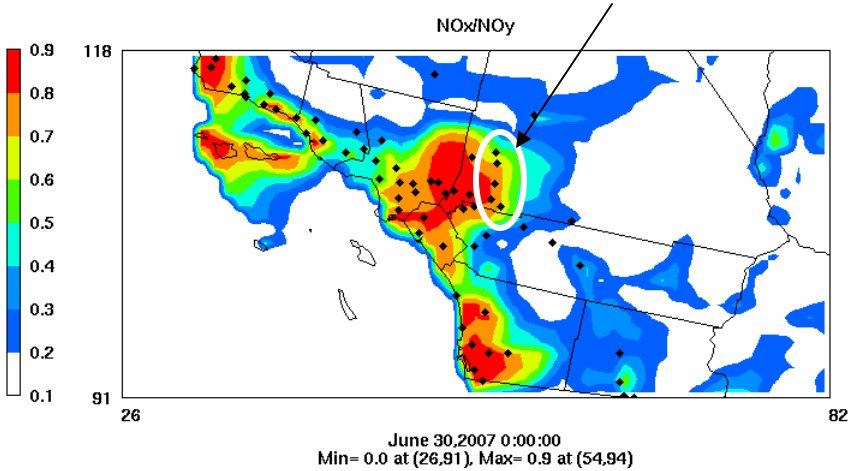
Low O_3 downwind
- in plume core

O_3 production at edge of the plume

High ratio suggesting modeled chemistry not evolving as rapidly as reality?

Large scale signature of urban NOx





LA Basin Performance: Are emissions too high?

NOx Emission Estimates in LA

tons/day

	On-road	Off-road	Stationary (area+point)	Total	Onroad/Offroad ratio
AQF Inventory	644	363	140	1147	1.77
CA AQMD 2002 Inventory	628	372	93	1093	1.68

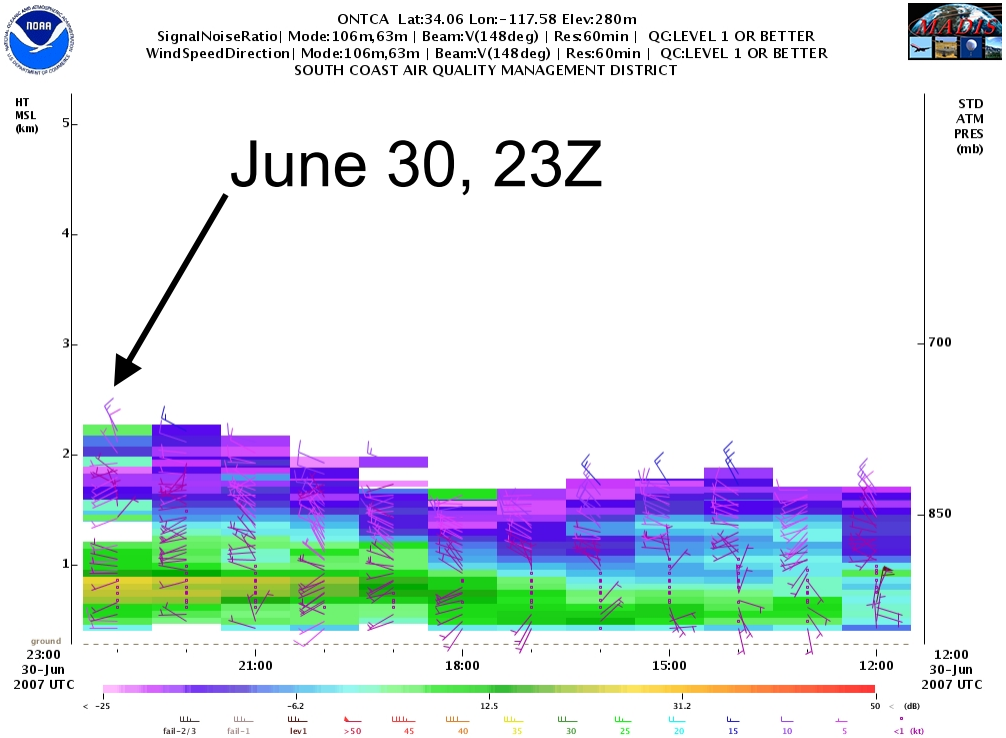
- CA AQMD estimates for South Coast Air Basin
- AQF Inventory estimates based on totals for 3 counties: ***Los Angeles, Orange, Riverside***

Reasonable agreement with 2002 AQMD estimates

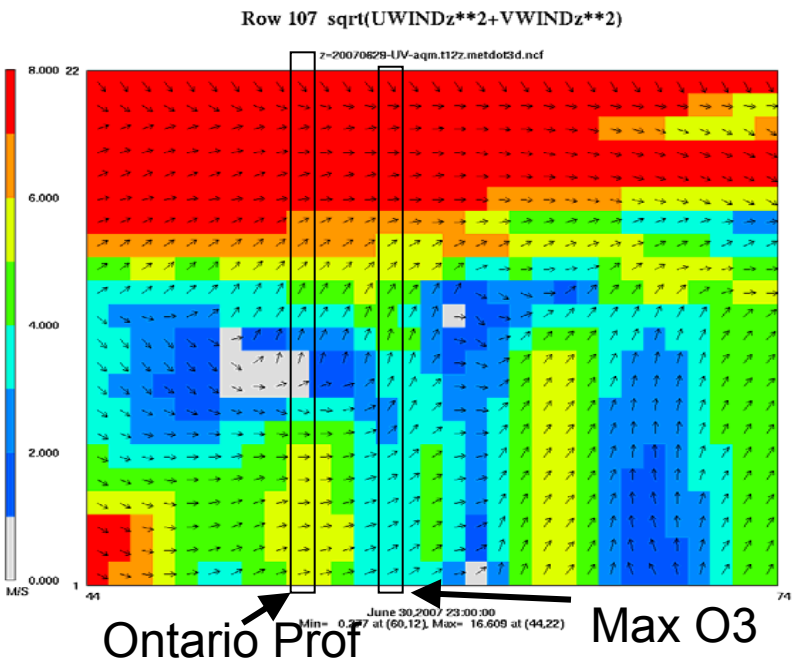
Have emissions in LA basin changed significantly in the 2002-2007 period?

Are wind speeds too high?

Time Ht Profile at Ontario



E-W Cross-section thru LA basin

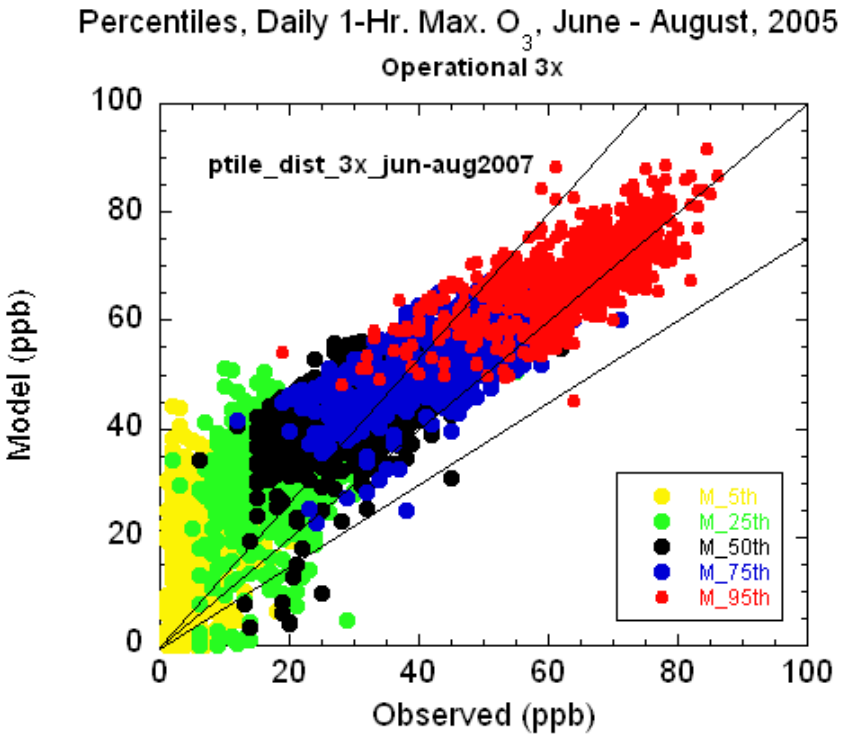


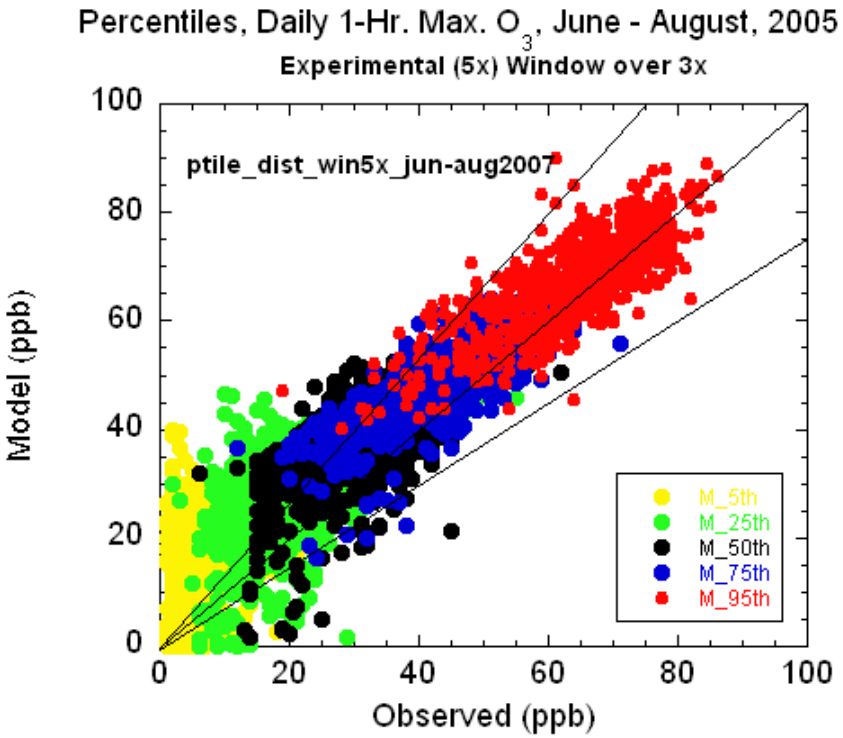
Modeled wind speeds appear to be stronger than those suggested by the profiler

- **Terrain induced flow may not be well represented**
  - **Flow patterns are complex in the LA Basin**
    - **Could impact how pollutants mix and thus impact model's representation of downwind chemical evolution**
    - **PDF of observed O3 suggest that intra-day forcing in CA is much stronger than that compared to sites in eastern U.S.**

Have model changes resulted in performance improvements?

Comparison of Operational and Experimental Configurations over Eastern U.S





In experimental configuration, over-predictions are reduced at all concentration ranges, especially at median, 75th, and 95th percentiles

Have model changes resulted in performance improvements?

Comparison of Operational and Experimental Configurations over Eastern U.S

Lower Bias

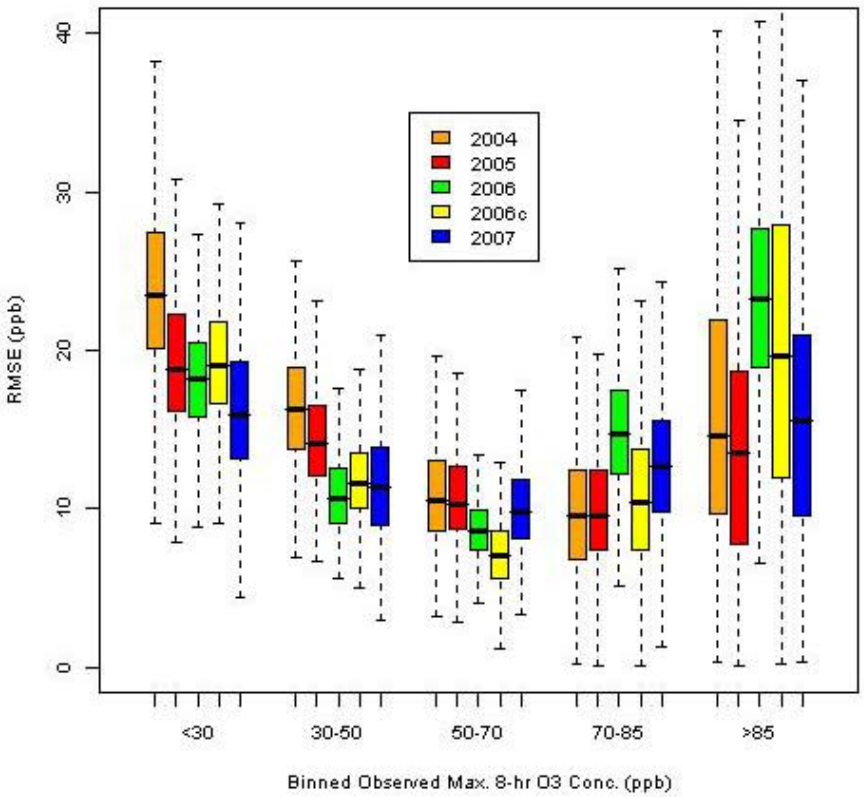
Lower Error

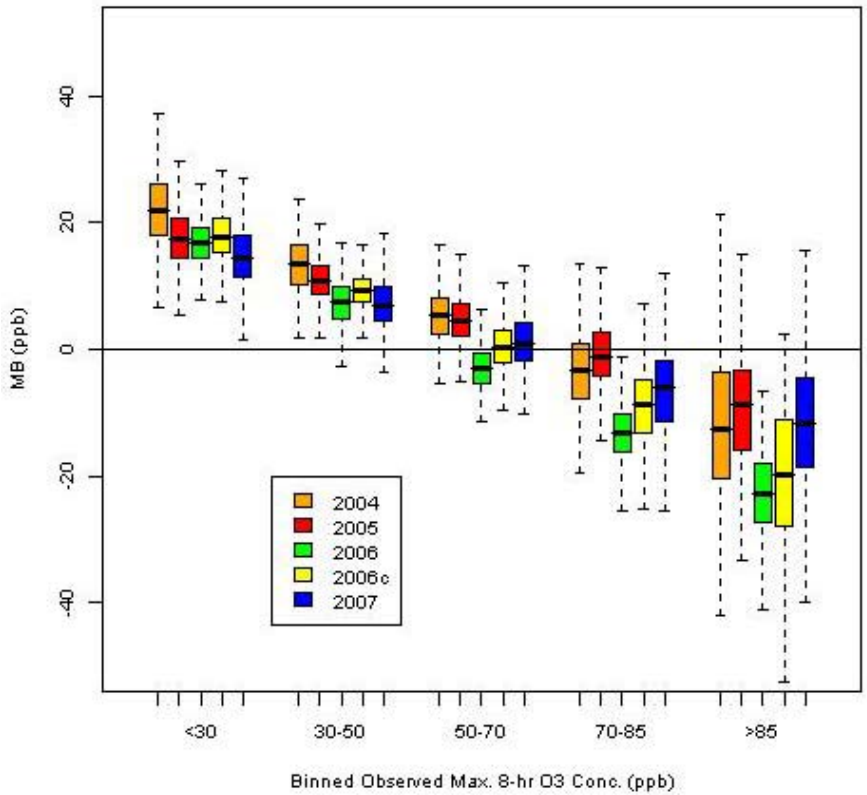
Higher Correlation

Have model changes resulted in performance improvements?

Mean-bias and RMSE at different concentration ranges; East U.S. sites; Experimental Configs.

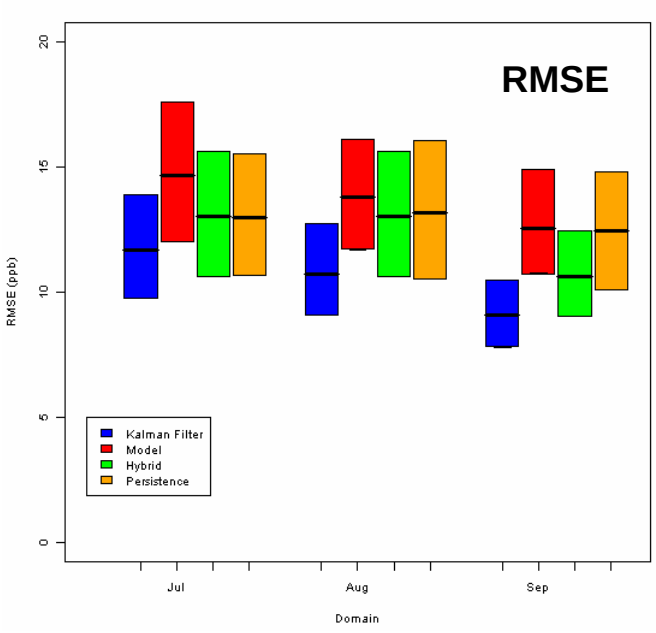
Note: 2006c represents data after correction of isoprene emission error





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

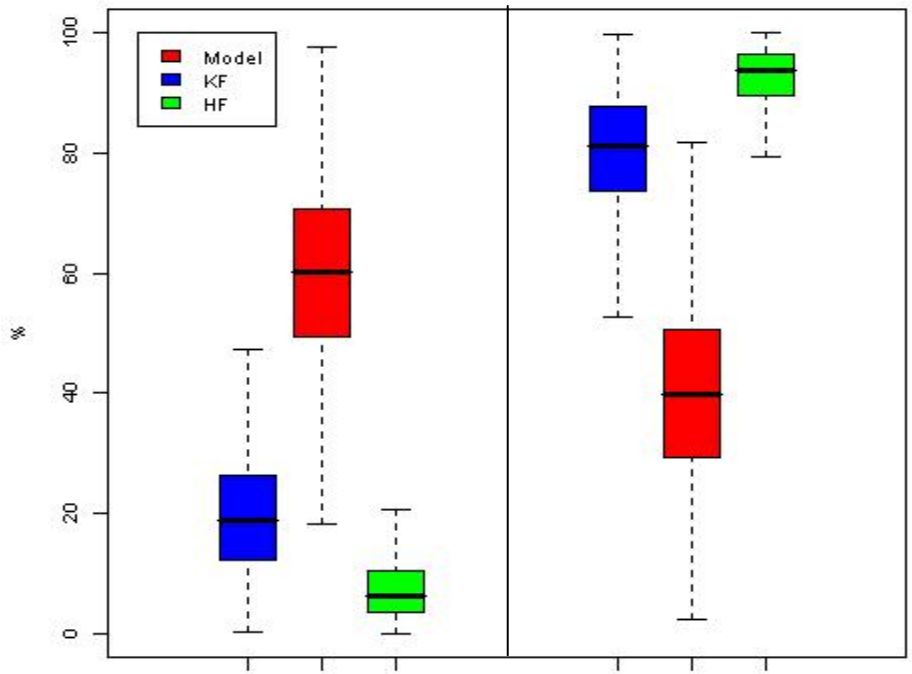
Looking ahead: Application of Bias-adjustment to forecasts



➡ ***Improves performance relative to both base model and a persistence forecast***

Methods Tested

- **"Hybrid" Forecast**: $HF_{t+\Delta t} = O_t + (M_{t+\Delta t} - M_t)$
- **Kalman Filter Predictor Bias Correction**



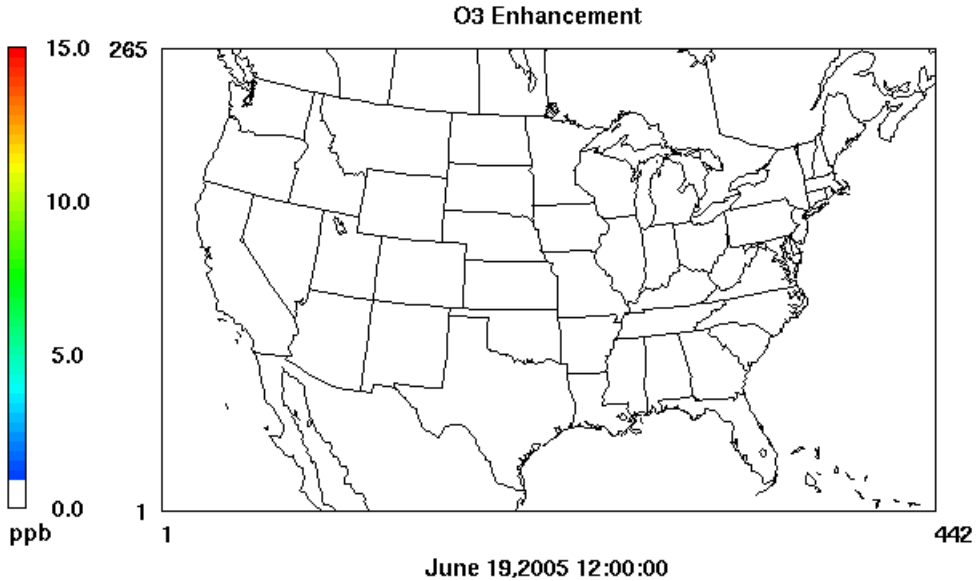
MSEs ***Systematic***

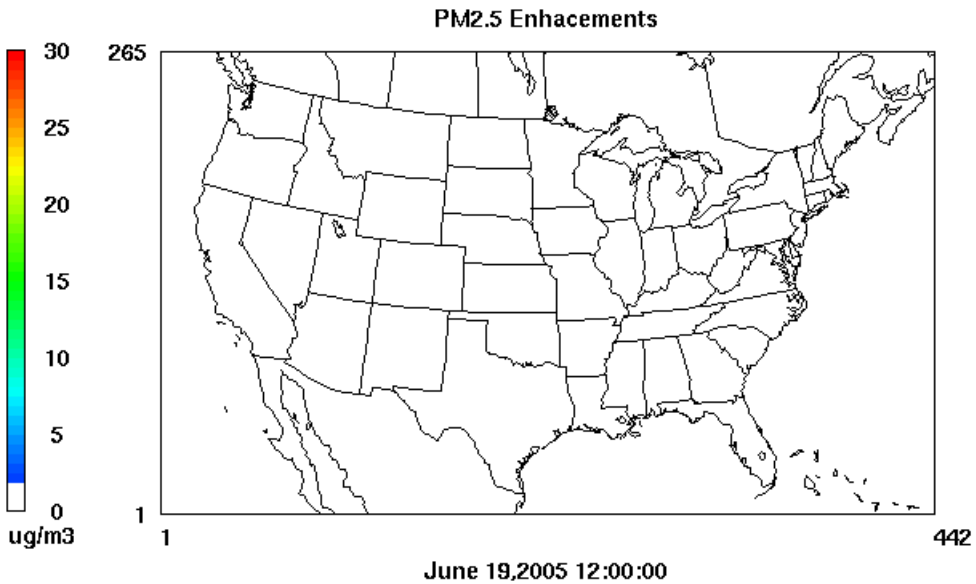
MSEu ***Unsystematic***

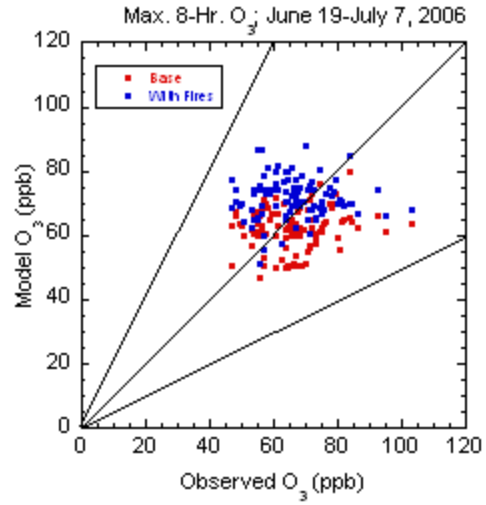
➡ ***Bias-adjustment can reduce the systematic errors but not the unsystematic component which represents the inherent random component in the measurements.***

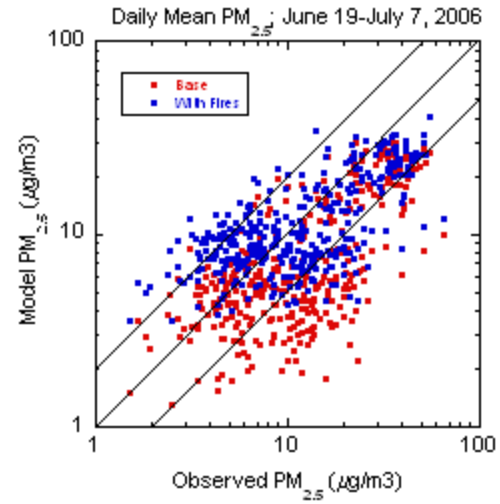
Looking ahead: Specification of "Real Time" Fire Emissions

Testing HMS-HYSPLIT fire emissions algorithm







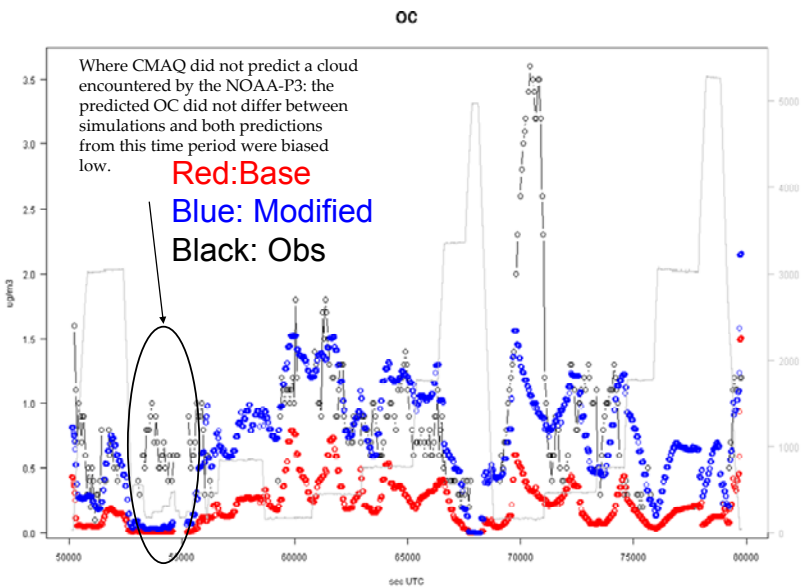


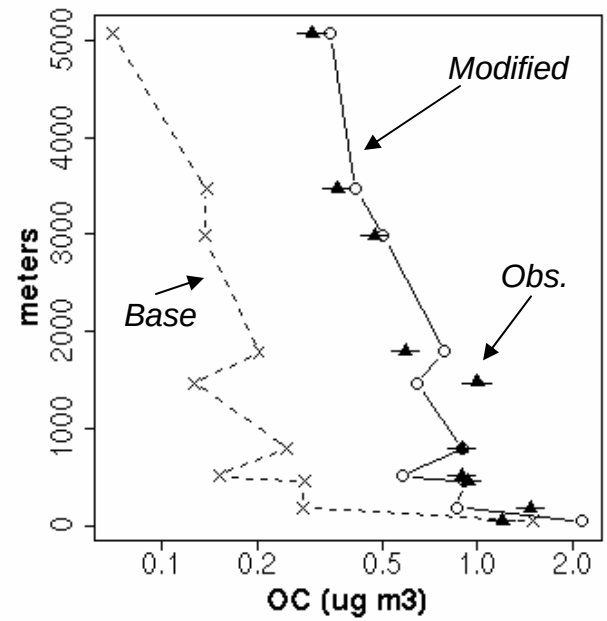
Accurate representation of wildfire emissions is important for both O_3 and PM forecasts

Looking ahead: Improvements in CMAQ PM model

Inclusion of in-cloud oxidation (GLY, MGLY) for SOA formation

Comparisons with NOAA-P3 measurements: August 14, 2004





Other on-going developments

- New SOA Module (pathways from aromatics, sesquiterpenes, isoprene oxidation)
  - *address summer-time low-bias*
- Improvements in representation of N_2O_5 hydrolysis
  - *address winter-time high-bias*
- Inclusion of sea-salt emissions and chemically active coarse mode

Summary

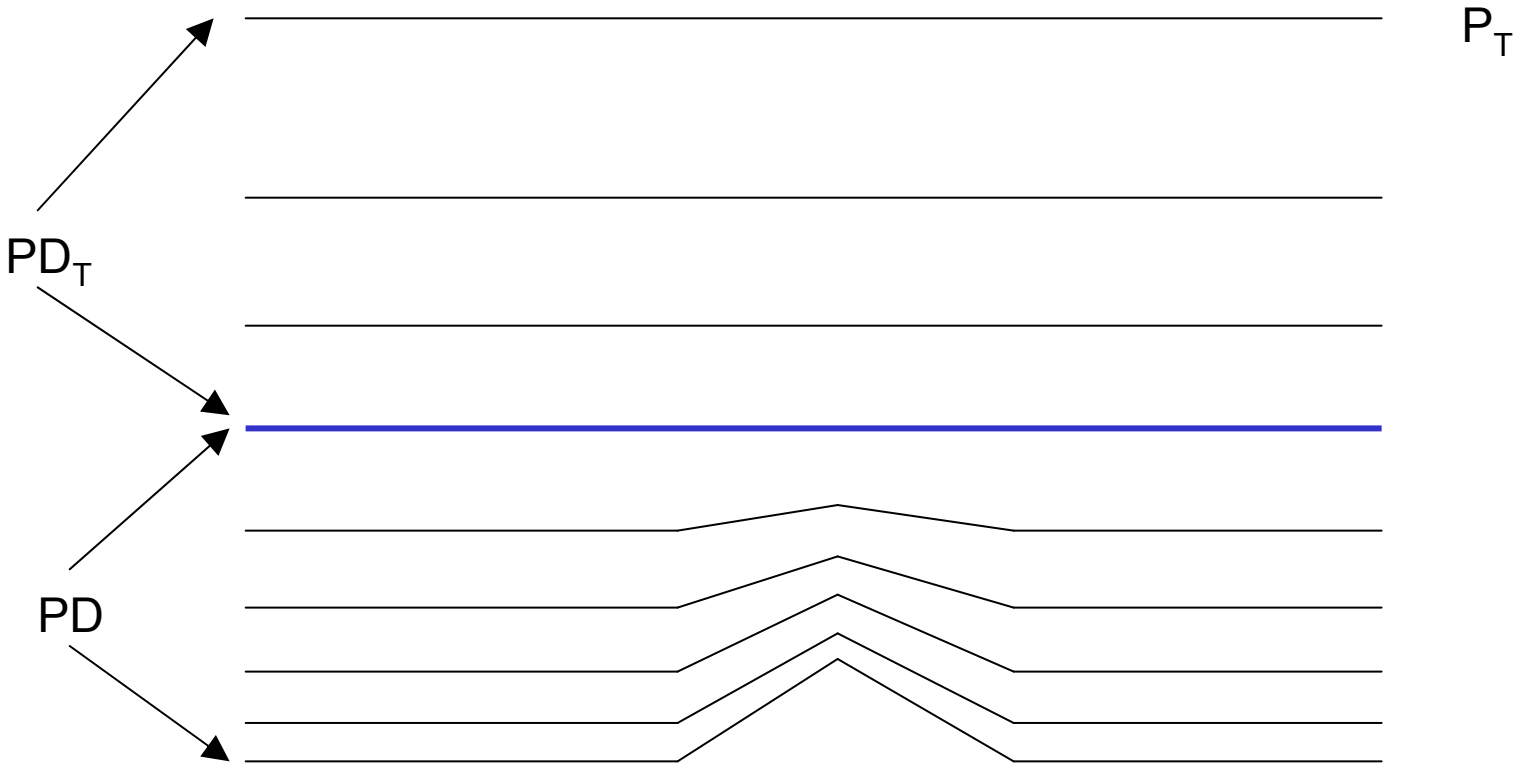
- AQF system transitioned to WRF-NMM in 2006/2007
  - Steady improvements in O_3 forecasts resulting from improvements in NAM, CMAQ, and their linkage
  - Performance of experimental configuration consistently better than operational model
  - Under-predictions in early May related to error in Mobile emissions
- Forecast performance in California (especially Central Valley) improved relative to previous years
  - Expansion of the operational domain to include Continental U.S.
  - Challenges in LA basin
- Diagnostic performance evaluations of developmental PM forecasts underway
  - Speciated data from STN, IMPROVE, CASTNET, SEARCH, TexAQS-2006
  - Investigation of upgrades to CMAQ PM module are underway

Backups

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

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)