United States Environmental Protection Agency

The Community Multi-scale Air Quality (CMAQ) Modeling System:

Past, Recent Developments, and New Directions

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Background

- ***The impact of human-induced perturbations on the chemical state of the atmosphere has received significant attention during the last two decades:***
  - Acid deposition, elevated tropospheric ozone, direct/indirect radiative effects of aerosols, greenhouse gases

- Scientific efforts to understand these have involved a combination of:
  - **Laboratory Experiments**
    - Provide basic data on individual physical/chemical processes
    - Provide parameters used by models
  - **Field Experiments**
    - Study limited number of atmospheric processes under conditions in which a few processes are dominant
    - Snapshot of atmospheric conditions at a particular time and location
  - **Modeling Experiments**
    - Tools to integrate and synthesize our evolving knowledge of various atmospheric processes

Why do we need atmospheric models?

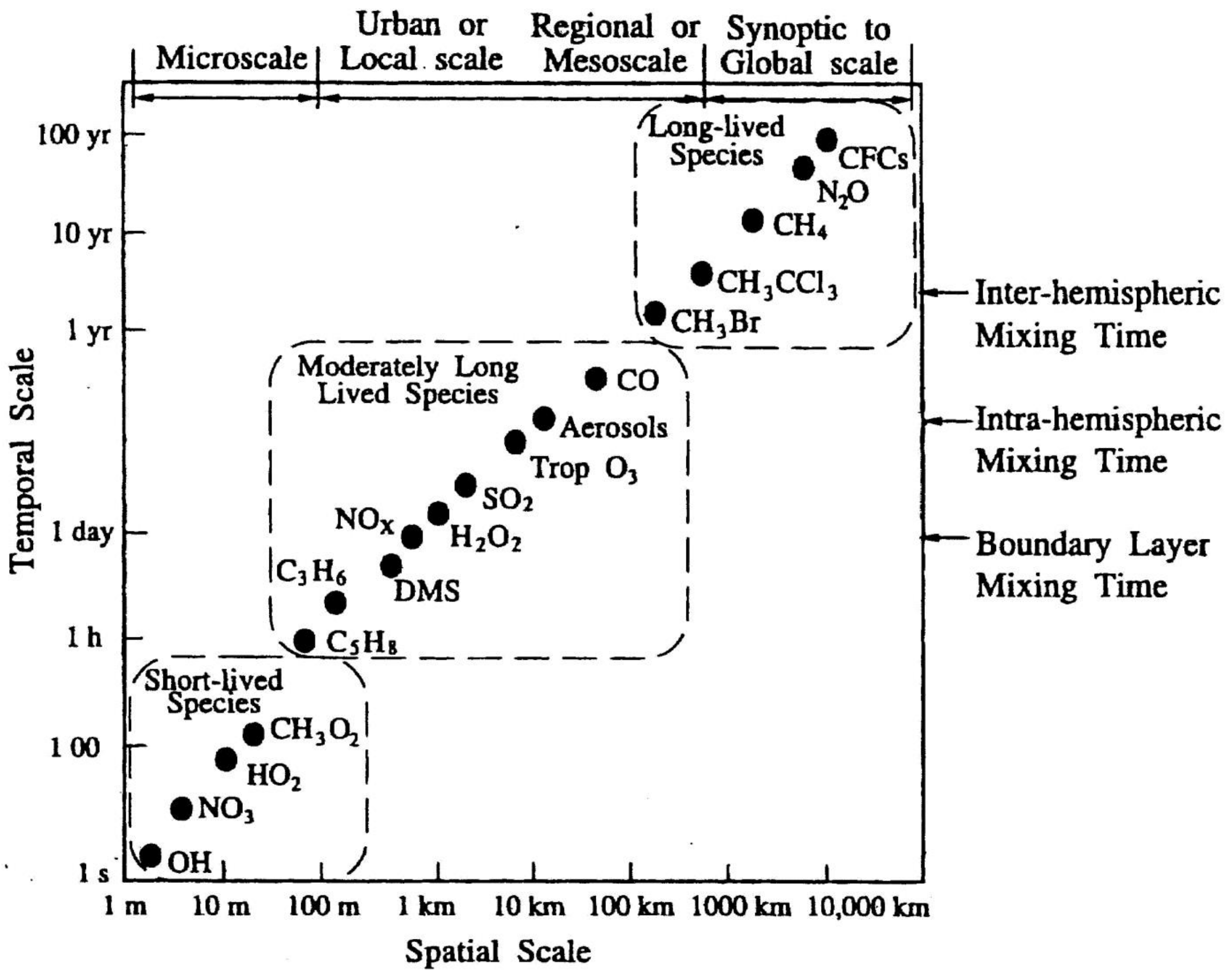
- The **complexity of physical and chemical atmospheric processes**, combined with the **enormity of the atmosphere**, make results obtained from laboratory and field experiments difficult to interpret without a **clear conceptual model of the workings of the atmosphere**, e.g.:
  - Extrapolation of results to other geographic areas
  - Assessing atmospheric chemical state in response to emission perturbations

- Because an understanding of individual processes may not necessarily imply an understanding of the overall system, measurements alone cannot be used to
  - Explore the future state of the atmosphere
  - Formulate effective abatement strategies

- Close integration of state-of-the-science models and experimental measurements is needed to advance our understanding of various atmospheric pollution problems

Atmospheric Pollutants

Space and Time-scales



Adapted from Seinfeld and Pandis

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Evolution of Air Quality Models

To address increasingly complex applications and assessments

Regulatory & Assessment Needs

- 1970 — CAA -Standards -Assessments
- 1977 — CAAA -PSD -New Source Permitting
- 1980 — NAPAP
- 1990 — CAAA
- 1994 — 1-hr O3 SIP
- 1997 — NAAQS 8-hr Oz PM 2.5
- 2000 — NATA & Air Quality Forecasting
- 2008 — SIPs Due - 8-hr Oz -PM - Hg -Toxics
- 2010+ — Climate & Air Quality Interactions; Exposure

1970 1977 1980 1990 1994 1997 2000 2004 2008 2010+

- AQDM
- UNAMAP
- RADM-ROM Eulerian Grid Models - Acid Deposition - Ozone
- MODELS3
- CMAQ For PM
- Neighbor Scale CMAQ - CFD - Eta-CMAQ
- Multi-pollutant CMAQ
- Coupled WRF-CMAQ

Single Pollutant
Non-reactive
Gaussian Dispersion
Local/urban Scales

Single Pollutant
Reactive
Eulerian Grid
Regional/urban Scales

Multi-pollutant
Multi-scale
Reactive
Eulerian Grid
Regional/urban Scales

Multi-pollutant
Multi-scale (***local to hemispheric***)
Interactions with Climate forcing and Air Quality changes
Reactive
Eulerian Grid

Model Development & Application

CMAQ Formulation: Equations

- The theoretical basis for model formulation is the **conservation of mass** for atmospheric trace species transport, chemistry, and deposition
- General form of chemical species equation:

$$\frac{\partial c_i}{\partial t} = \left(\frac{\partial c_i}{\partial t}\right)_{adv} + \left(\frac{\partial c_i}{\partial t}\right)_{diff} + \left(\frac{\partial c_i}{\partial t}\right)_{cloud} + \left(\frac{\partial c_i}{\partial t}\right)_{dry} + \left(\frac{\partial c_i}{\partial t}\right)_{aero} + R_{gi} + E_i$$

$\left(\frac{\partial c_i}{\partial t}\right)_{adv}$ Rate of change of c_i due to advection

$\left(\frac{\partial c_i}{\partial t}\right)_{diff}$ Rate of change of c_i due to turbulent diffusion

$\left(\frac{\partial c_i}{\partial t}\right)_{cloud}$ Rate of change of c_i due to cloud processes (*scavenging, evaporation, aqueous chemistry, wet deposition*)

$\left(\frac{\partial c_i}{\partial t}\right)_{dry}$ Rate of change of c_i due to dry deposition

$\left(\frac{\partial c_i}{\partial t}\right)_{aero}$ Rate of change of c_i due to aerosol processes (*interphase transfer between gas and aerosol, aerosol dynamics*)

CMAQ Formulation

Modular, Generalized, and Extensible

Generalized Coordinate Formulation

$$\frac{\partial \varphi_i^*}{\partial t} + \hat{\nabla}_\xi \bullet \left[\varphi_i^* \hat{\overline{\mathbf{V}}}_\xi\right] + \frac{\partial(\varphi_i^* \overline{\hat{v}^3})}{\partial \hat{x}^3} + \hat{\nabla}_\xi \bullet \left[\overline{\rho}\sqrt{\hat{\gamma}}\hat{\mathbf{F}}_{q_i}\right] + \frac{\partial(\overline{\rho}\sqrt{\hat{\gamma}}\hat{F}^3_{q_i})}{\partial \hat{x}^3}$$

horizontal advection · *vertical advection* · *horizontal diffusion* · *vertical diffusion*

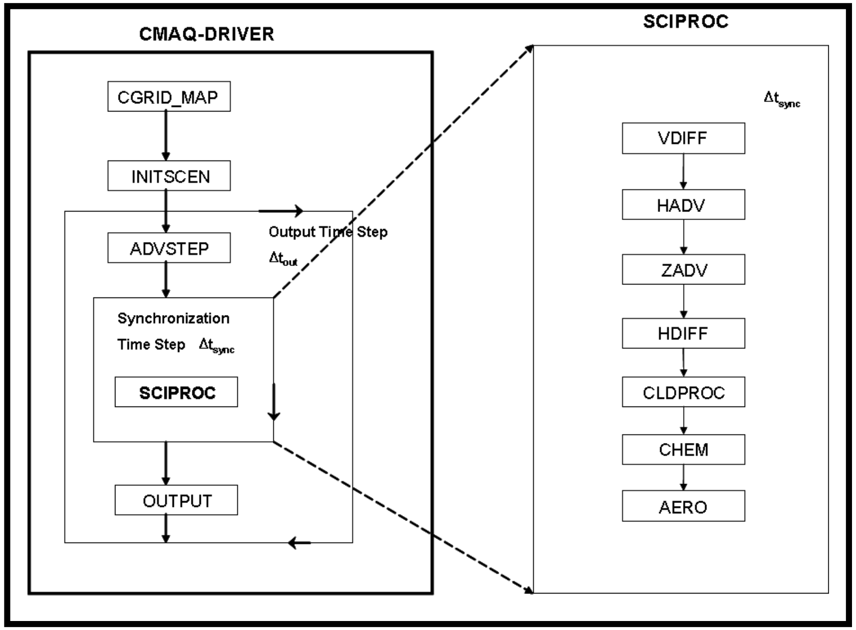
$$= \sqrt{\hat{\gamma}} R_{\varphi_i}(\overline{\varphi}_1, \ldots, \overline{\varphi}_N) + \sqrt{\hat{\gamma}} S_{\varphi_i} + \left.\frac{\partial(\varphi_i^*)}{\partial t}\right|_{cld} + \left.\frac{\partial(\varphi_i^*)}{\partial t}\right|_{aero}$$

chemistry · *emissions* · *clouds* · *aerosols*

where, $\varphi_i^* = \sqrt{\hat{\gamma}}\,\overline{\varphi}_i = (J_\xi / m^2)\overline{\varphi}_i$

$\sqrt{\hat{\gamma}}$ encapsulates coordinate transformation from physical to computational space

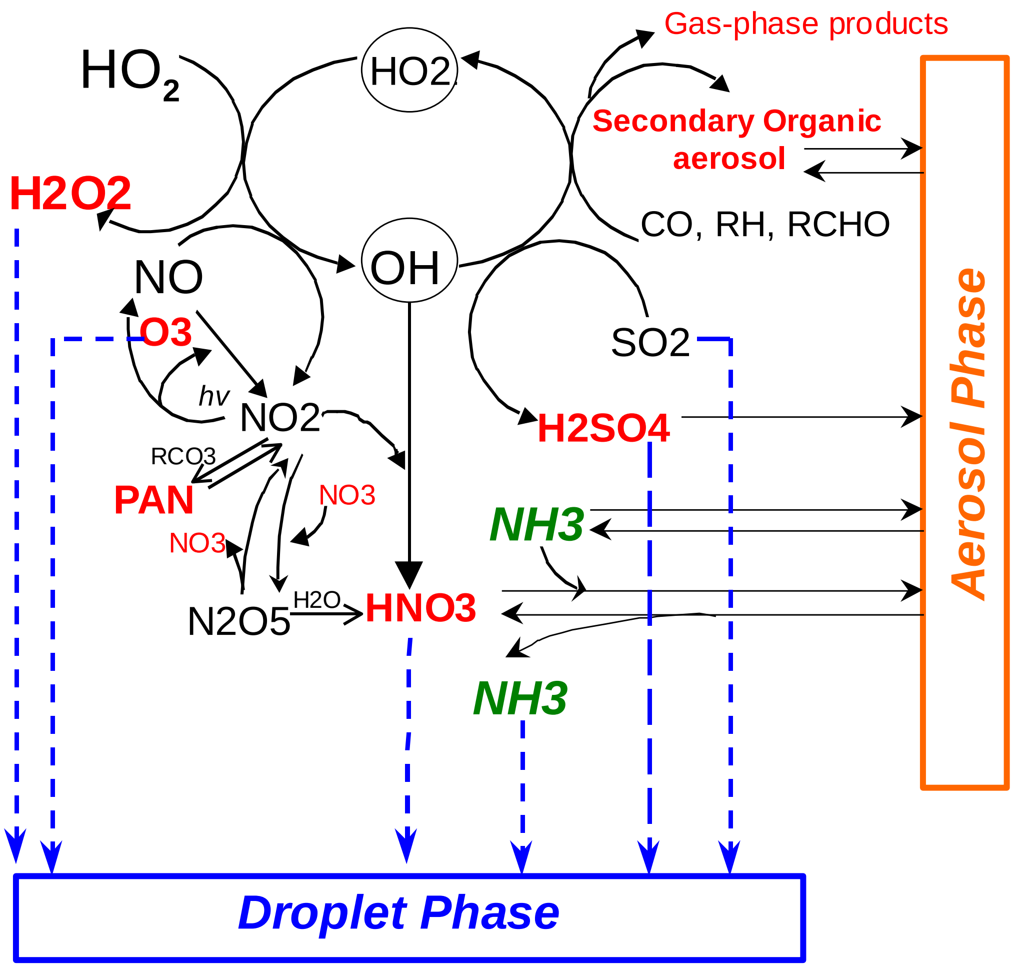
Solution Method: Fractional Steps



Accounting for Process Interactions

Example: Gas-Aqueous-Aerosol Phase Chemistry

The NO_x-SO_x-NH_x System



Atmospheric fate and lifetimes of reduced and oxidized nitrogen are linked

Adapted from : Meng et al. (1997); Warneck (1988)

CMAQ Modeling System

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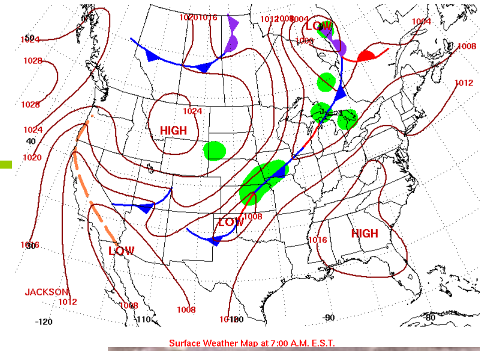
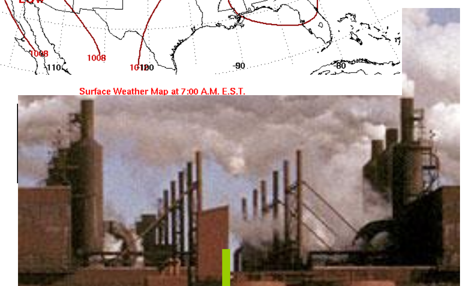
Meteorological Model (WRF)





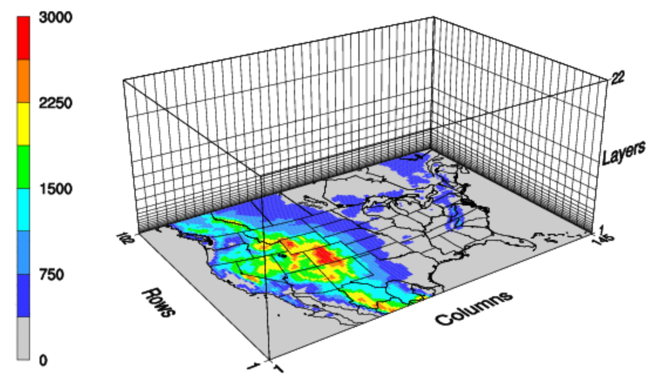
Meteorological-Chemical Interface Processor (MCIP) (AQPREP)

SMOKE

Anthropogenic and Biogenic Emissions processing

CMAQ AQ Model-

Chemical-Transport Computations



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The Community Multiscale Air Quality (CMAQ) model:

- **Eulerian** grid chemical transport model
- **Multi-scale**: Hemispheric → Continental →Regional → Local
- **Multi-pollutant**:
  - **Ozone Photochemistry**
    - NO_x + VOC (biogenic & anthropogenic) →O_3
  - **Particulate Material (PM)**
    - Inorganic chemistry & thermodynamics → Sulfate, Nitrate, Ammonium
    - Organic aerosol → primary, secondary
  - **Acid deposition**
    - Aqueous chemistry, Wet deposition
  - **Air Toxics**
    - Benzene, Formaldehyde, Hg, etc
- **Community Model**
  - First version publicly released in ~2000
  - CMAQv5.0 released in February 2012

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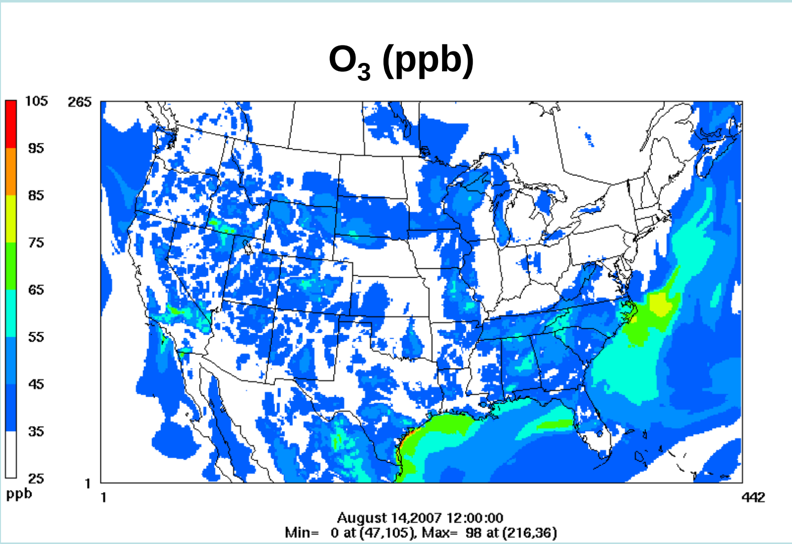
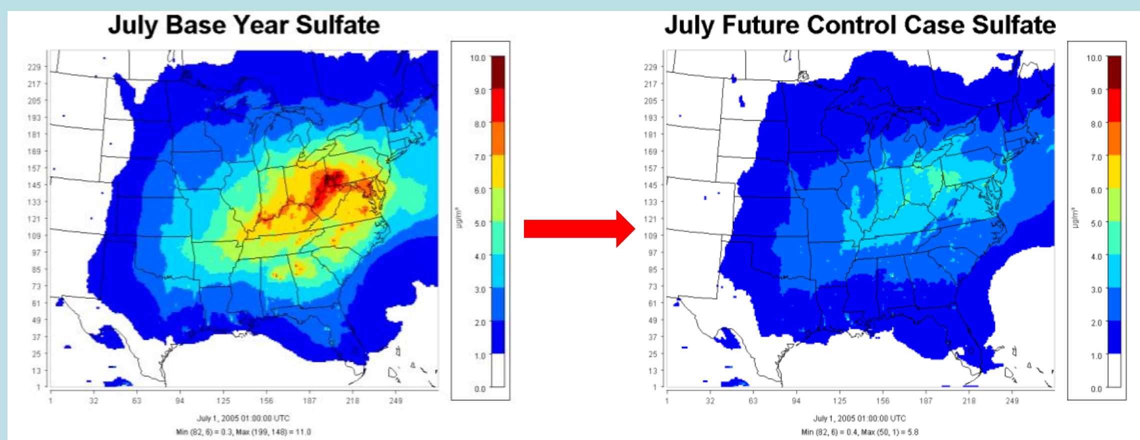
Typical Regional-Scale CMAQ Applications



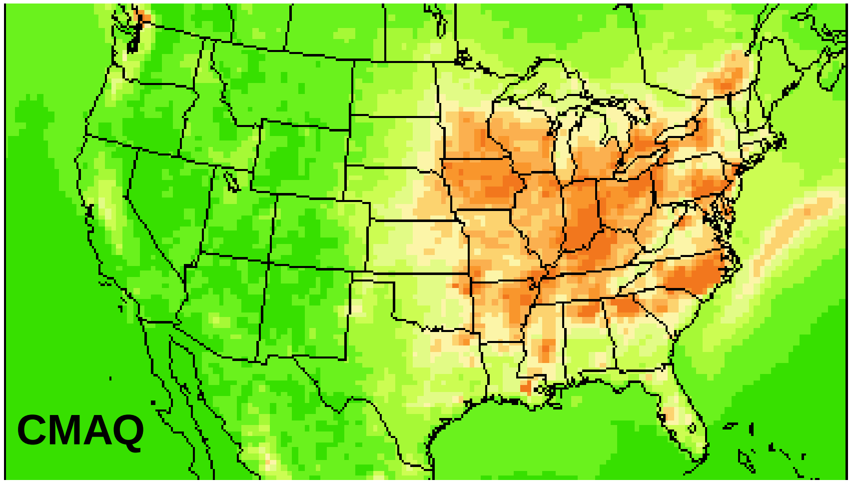
Regional-scale air quality modeling studies (time-scales ranging from days to years)

Simulating the effectiveness of emission control strategies

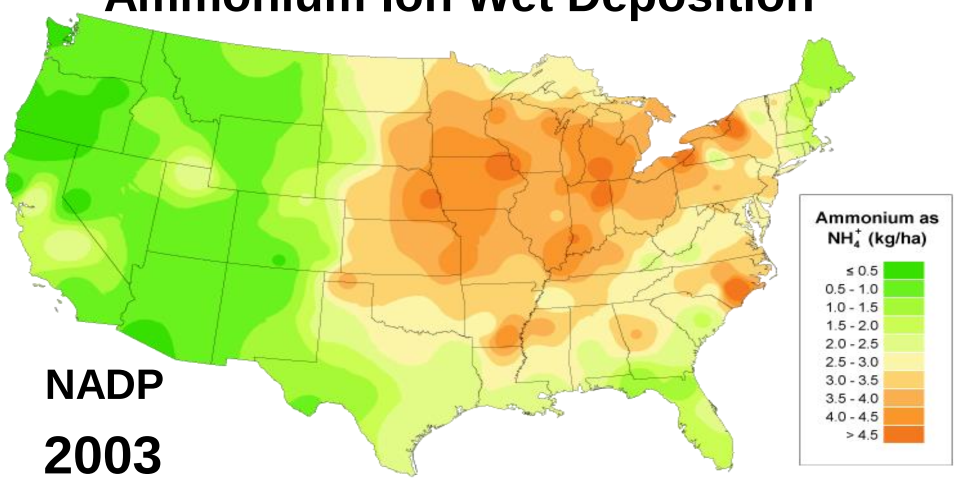


CMAQ Applications: Atmospheric N Depositions

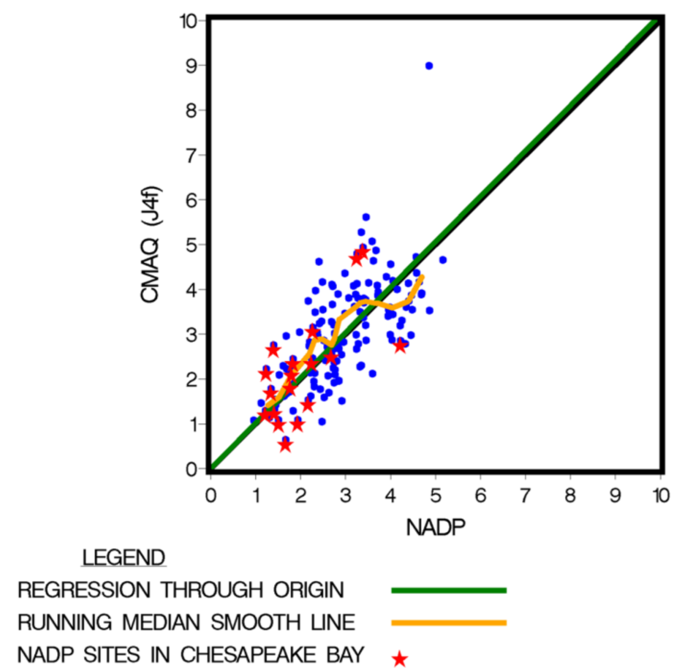
Nutrient loading to sensitive Ecosystems



Ammonium Ion Wet Deposition



WET NH4 DEPOSITION (KG/HA)
CMAQ (J4f)
VS. NADP (2001–2003 AVERAGED)
LIMITED TO SITES IN THE EASTERN U.S.
ANNUAL

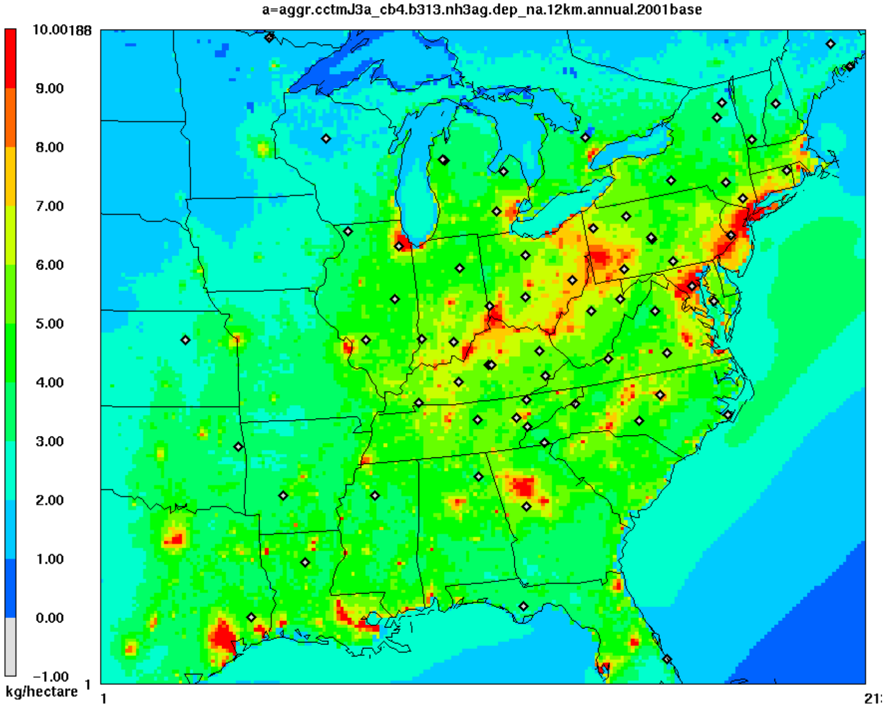


CMAQ is able to capture main spatial pattern and magnitude of wet deposition

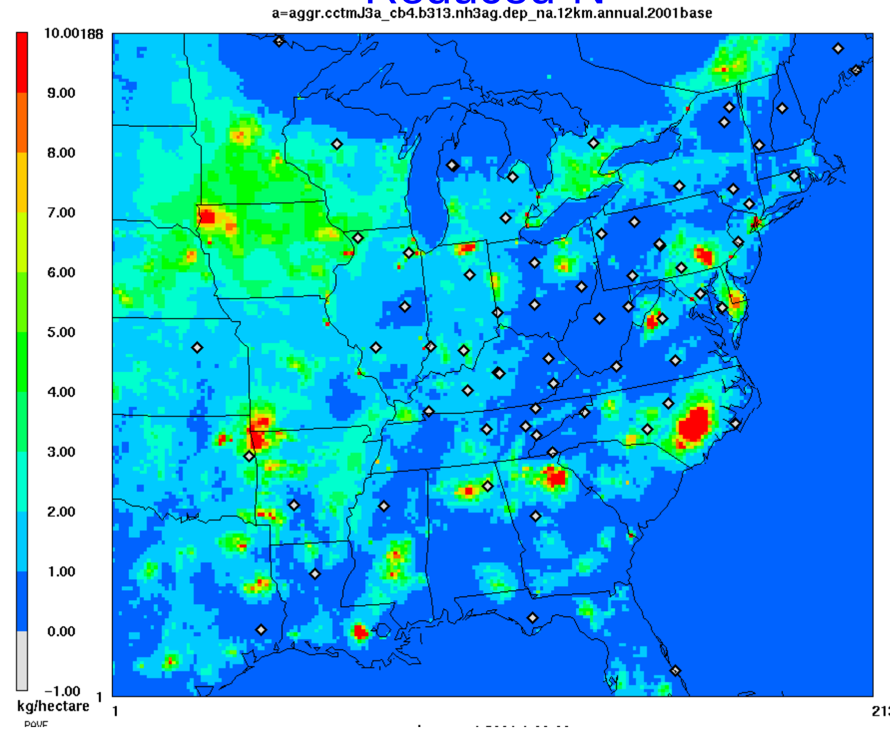
Defining Dry Deposition Monitoring Needs

Modeled spatial trends vs. CASTNET location

Oxidized-N



Reduced-N



Current coverage is not representative,
budget based on obs will be misleading

Need for greater spatial coverage

CMAQ Applications:
Developing Daily Air Quality Forecast Guidance

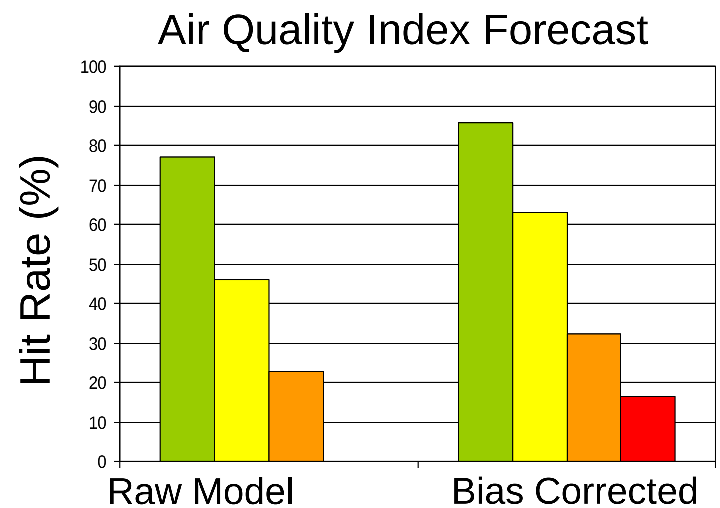
Observations +Meteorology +Models

Pollutant Concentrations

AIR QUALITY INDEX

200 Very Unhealthy
150 Unhealthy
100 Unhealthy for sensitive groups
50 Moderate
Good

State and Local Agencies



Bias correction can improve the forecast accuracy for the moderate to unhealthy AQI categories

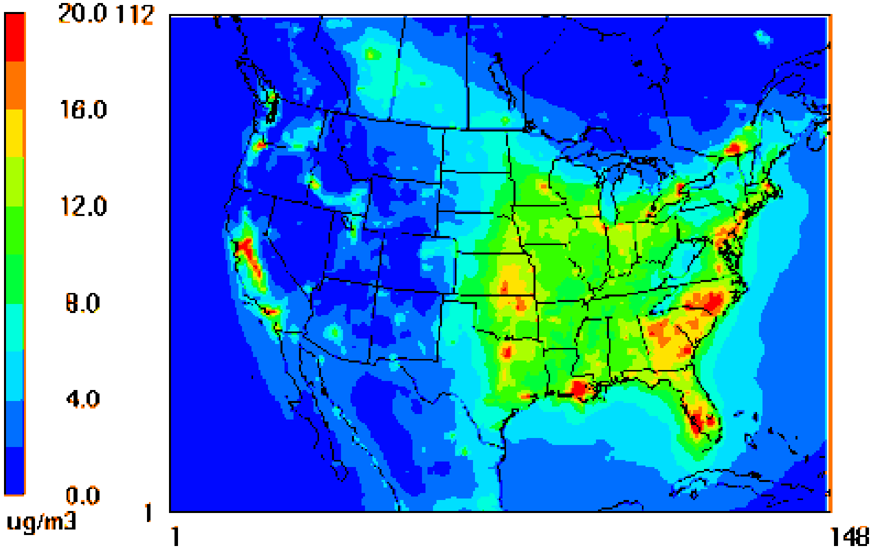
Sensitivity Analysis: Direct Decoupled Method

CMAQ-DDM-3D: an efficient and accurate approach for calculating first- and second-order sensitivity of atmospheric pollutant concentrations and accumulated deposition amounts to changes in photochemical model parameters (emissions, chemical reaction rates, initial/boundary conditions, etc.)

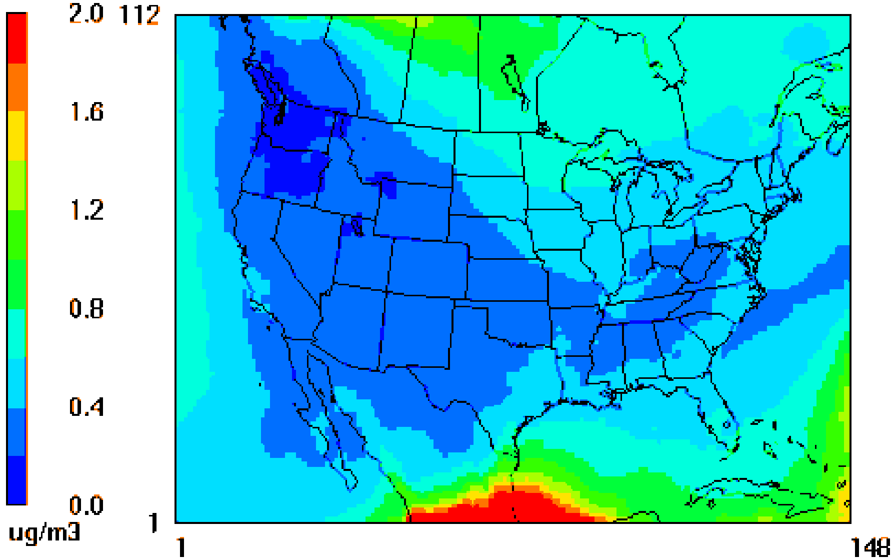
Sensitivity of species *i* to model parameter *j*:

$$\frac{\partial \mathbf{S}_{i,j}}{\partial t} = -\nabla\left(u\mathbf{S}_{i,j}\right) + \nabla\left(K\nabla\mathbf{S}_{i,j}\right) + J\mathbf{S}_{i,j} + E_i'$$

January $PM_{2.5}$



$PM_{2.5}$: LBC Contribution

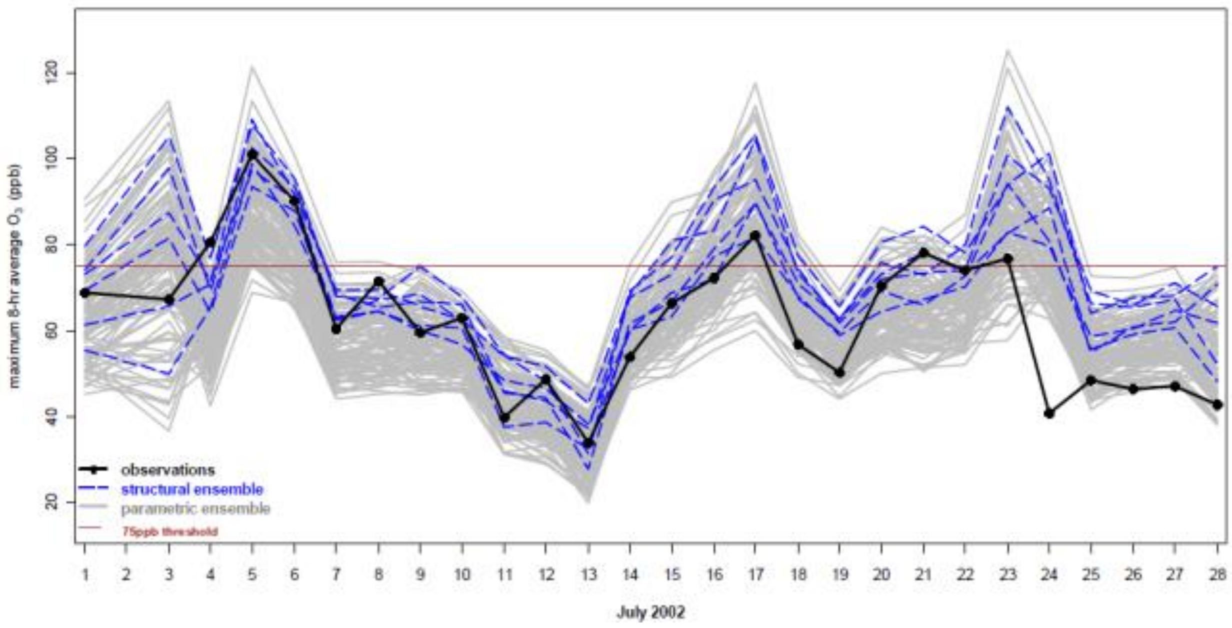


Courtesy: Sergey Napelenok

Propagating Uncertainty to Model Output

Reduced form model based on Taylor series: The response from fractional changes in the amounts of $\Delta\varepsilon_j$ and $\Delta\varepsilon_k$ to two model parameters *j* and *k* can be described as:

$$\mathbf{C}_{\varepsilon_j,\varepsilon_k} \approx \mathbf{C}_0 + \Delta\varepsilon_j S_j^{(1)} + \Delta\varepsilon_k S_k^{(1)} + \frac{\Delta\varepsilon_j}{2} S_{j,j}^{(2)} + \frac{\Delta\varepsilon_k}{2} S_{k,k}^{(2)} + \Delta\varepsilon_j \Delta\varepsilon_k S_{j,k}^{(2)}$$



Ensemble time series of CMAQ daily max 8-hr average ozone predictions at a monitoring site in downtown Atlanta for July 2002.

Courtesy: Kristen Foley

Emerging Needs:
Air Quality-Climate Interactions

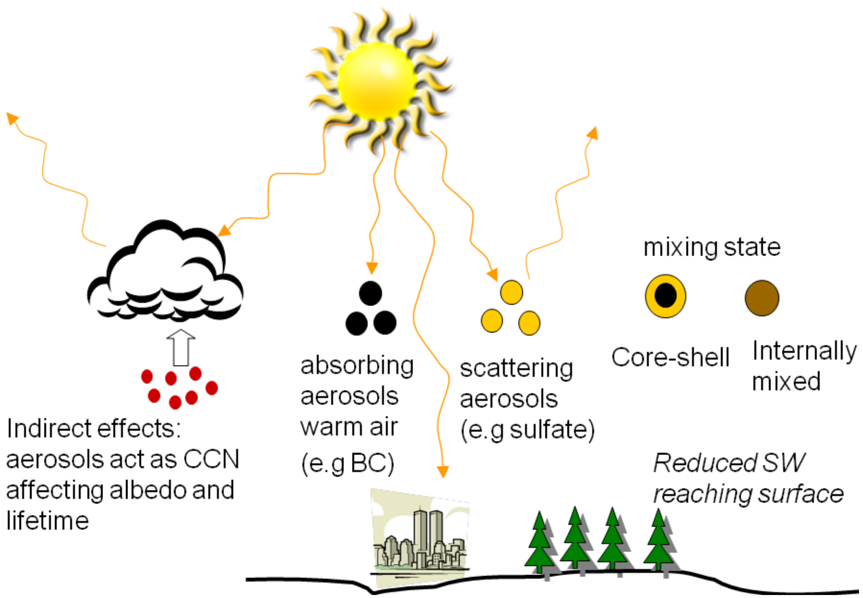
Beijing December 2011
3 pm; $PM_{2.5}$ ~ 260 $\mu g/m^3$

Picture Courtesy: Jon Pleim

Air Quality-Climate Interactions

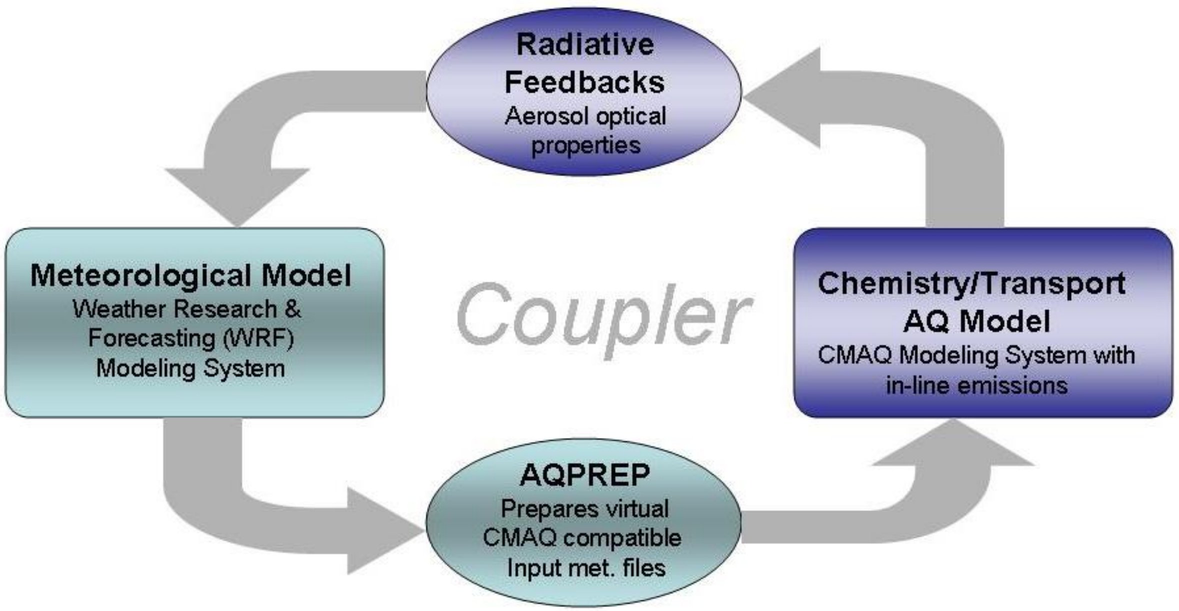
Optical and Radiative Characteristics of Aerosols

- **Direct effects**
  - **Light scattering aerosols** (e.g., sulfate)
    – Backscatter incoming solar
    Reduce radiation impinging on the Earth's surface
    ➡ *cool the surface (negative surface forcing)*
    Increase radiation reflected to space
    ➡ *cool the top of the atmosphere (negative TOA forcing)*
  - **Light absorbing aerosols** (e.g., BC)
    – Absorb incoming solar
    Reduce radiation impinging on the Earth's surface
    ➡ *cool the surface (negative surface forcing)*
    – Absorb outgoing solar reflected from surface and clouds
    ➡ Reduce radiation reflected to space
    Warm the top of the atmosphere (positive TOA forcing)



- **Indirect effects**
  – Changes in cloud formation and duration resulting from scattering and absorption
  – Aerosols act as CCN; impact cloud optical thickness; impact cloud lifetime

Two-Way Coupled WRF-CMAQ Modeling System:
Design and Model Features



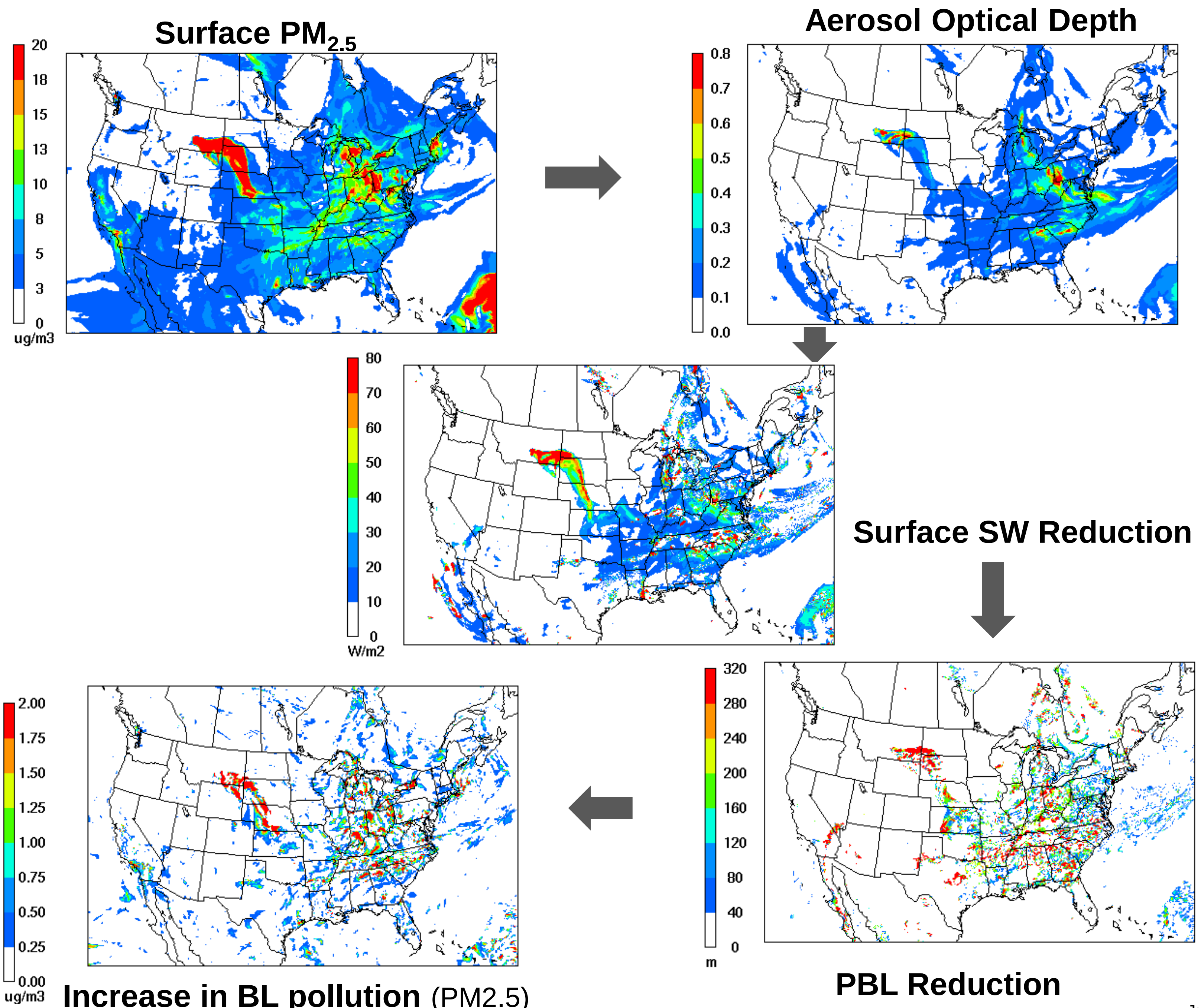
Aerosol Optics & Feedbacks

- Volume weighted refractive indices for each wavelength based on
  - Composition and size distribution
  - SO_4^{2-}, NO_3^-, NH_4^+, Na^+, Cl^-, EC, POA, anthropogenic and biogenic SOA, other primary, water
- Both RRTMG and CAM Shortwave radiation schemes in WRF
- Effects of aerosol scattering and absorption on photolysis
- Effects of O_3 on long-wave radiation

Flexible **design of model coupling allows**

- data exchange through memory resident buffer-files
- flexibility in frequency of coupling
- identical on-line and off-line computational paradigms with minimal code changes
- both WRF and CMAQ models to evolve independently;

➡ *Maintains integrity of WRF and CMAQ*

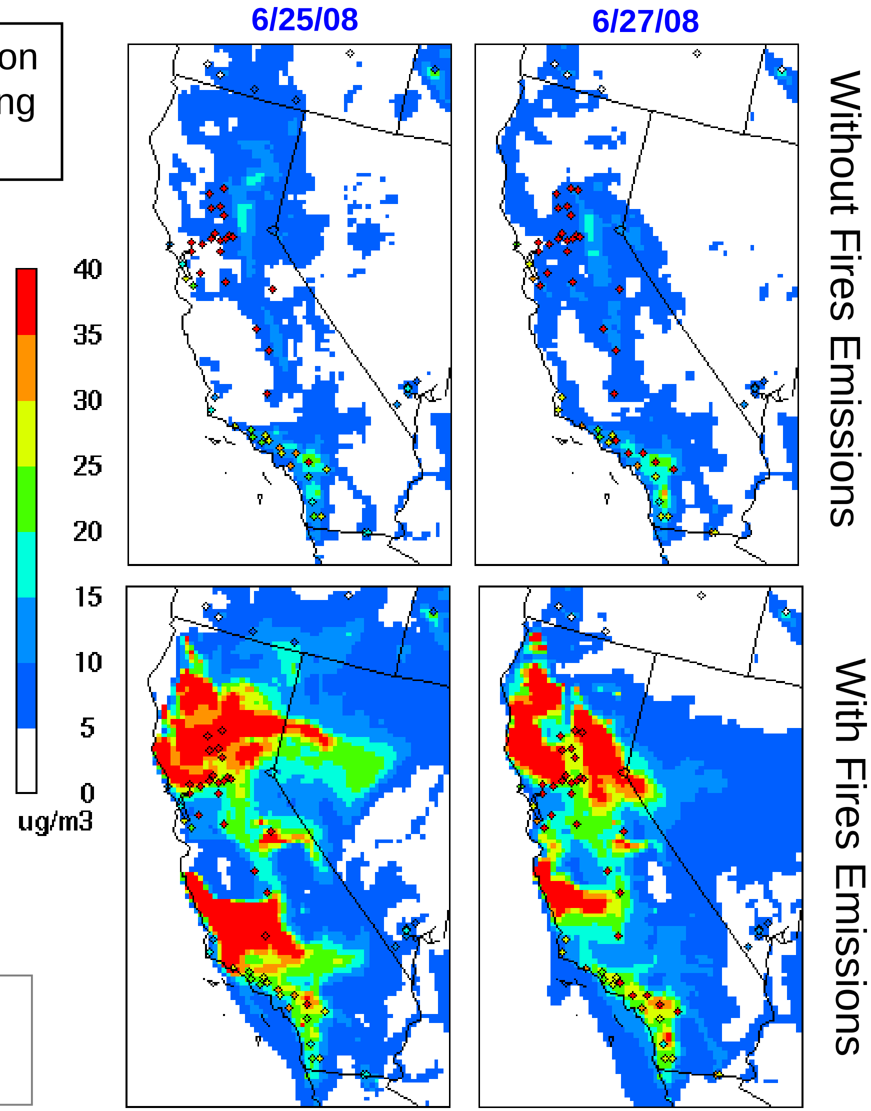


July 14, 2006 21Z

California Wildfires

A High Aerosol Loading Case

Widespread wildfires resulted in significant PM pollution during mid/late June 2008 in California and surrounding states



Daily-avg. $PM_{2.5}$

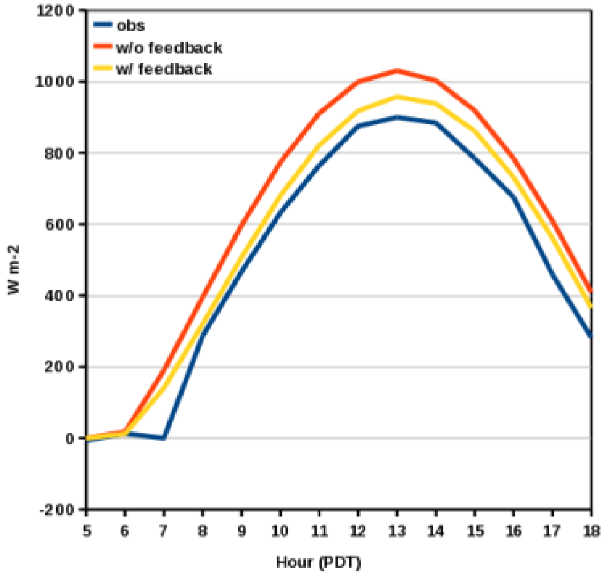
- Fuel loading: National Fire DangerRating (NFDR) system
- Emission Factors: Fire Emission Production Simulator (FEPS) Function of fuel class

Shortwave Radiation Reaching the Surface

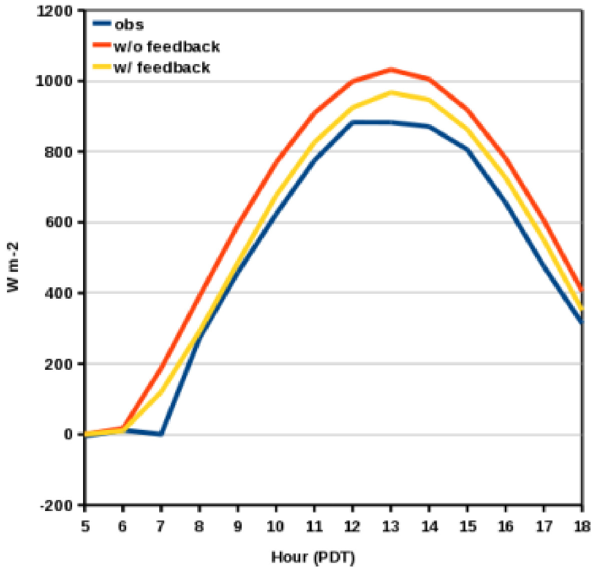
With and Without Feedbacks

Comparison with measurements at ISIS site at Hanford, CA

June 26



June 27

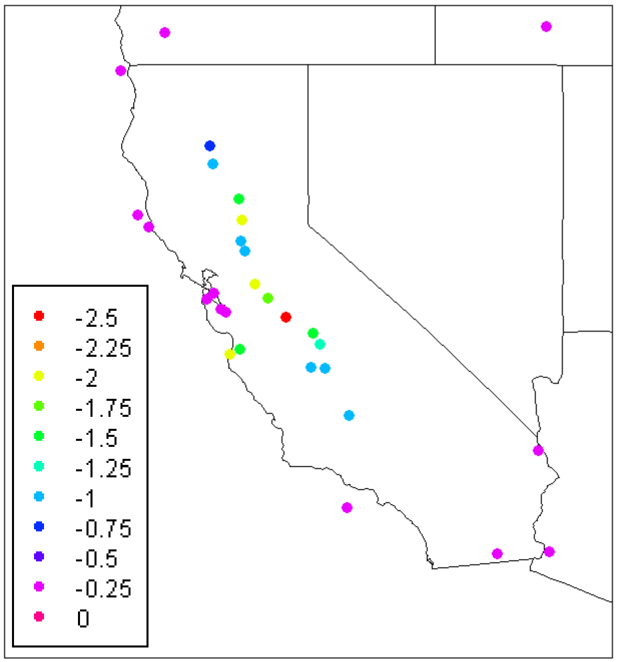


- More pronounced reduction in shortwave radiation due to aerosol loading
- Including aerosol direct forcing improves simulation of SW radiation

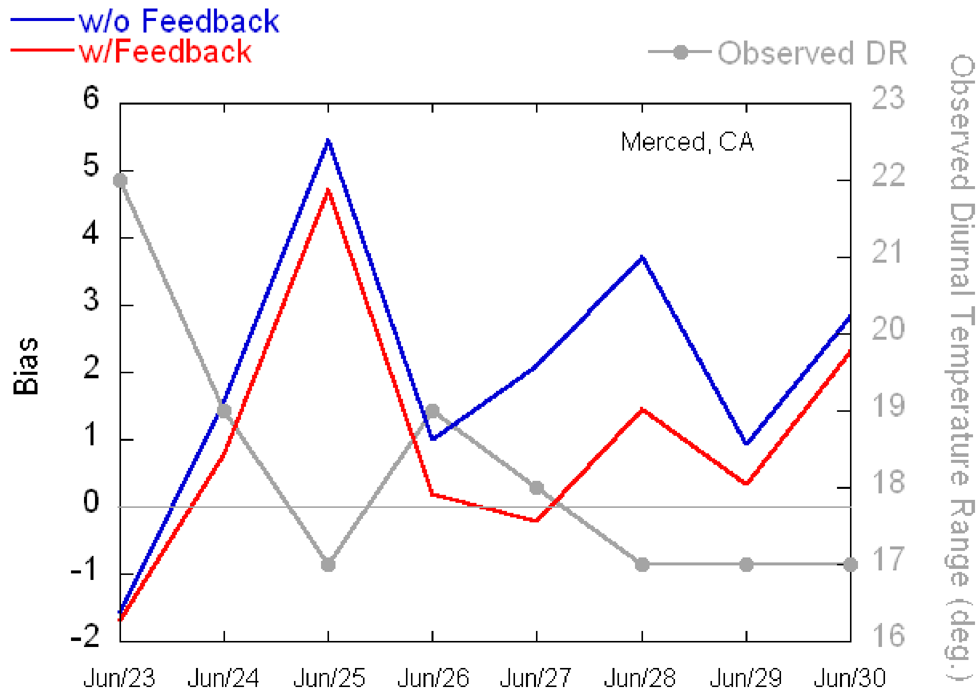
Diurnal Temperature Range (DTR)

Proxy for variability in surface solar radiation

Difference in DTR
w/Feedback – w/o Feedback
June 28, 2008



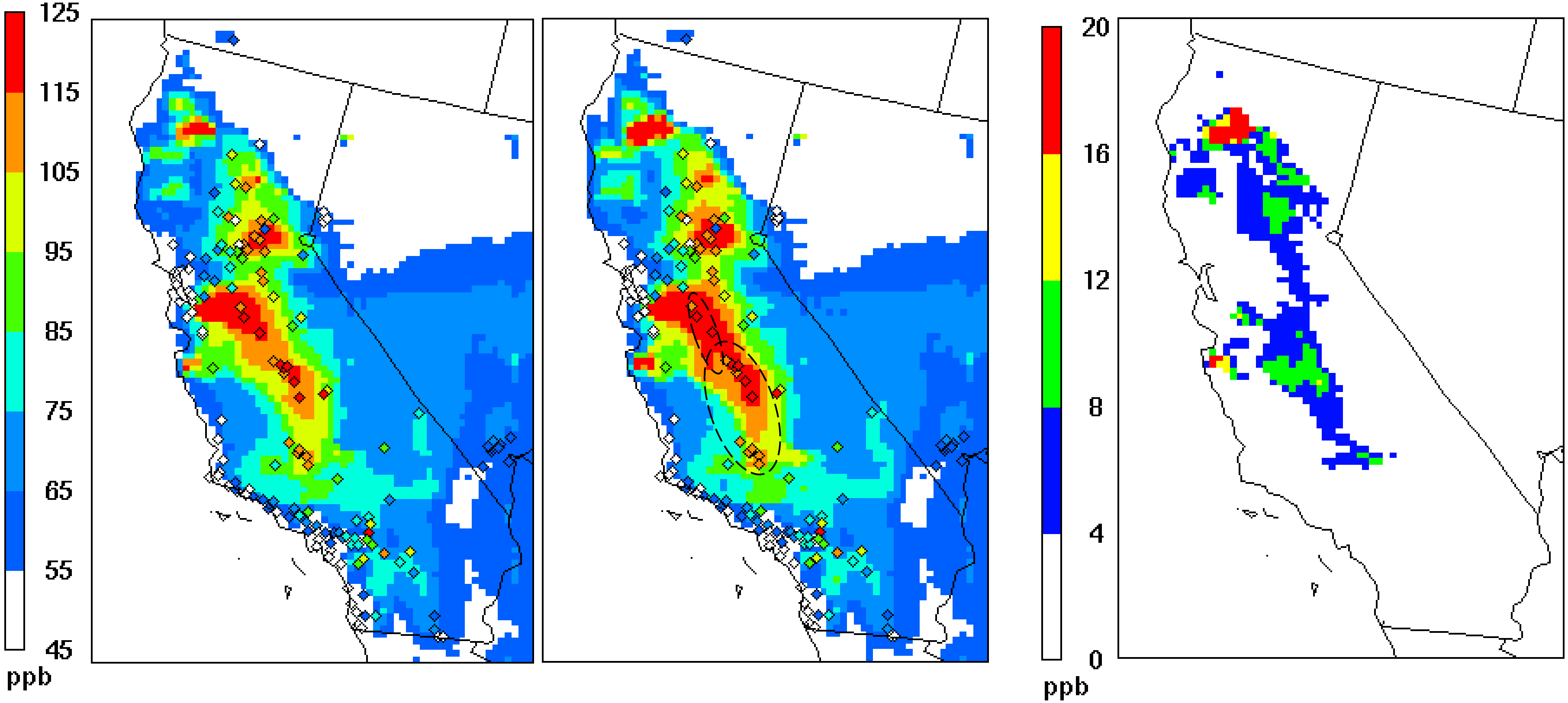
Comparison with observed range at site impacted by wildfire plume



Reduction in bias in simulated DTR

- **More widespread observations of DTR could be used to assess aerosol effects**

Maximum 8-hr. O_3: June 27 2008



Without Feedbacks

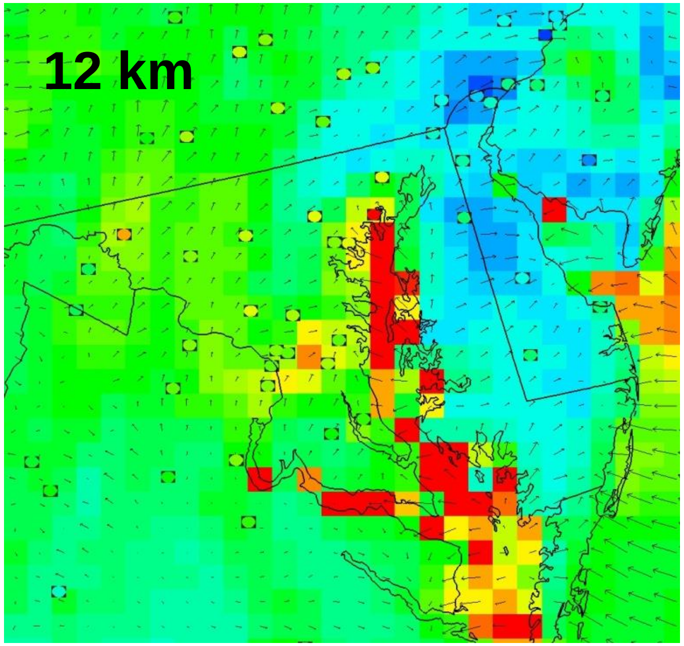
With Feedback

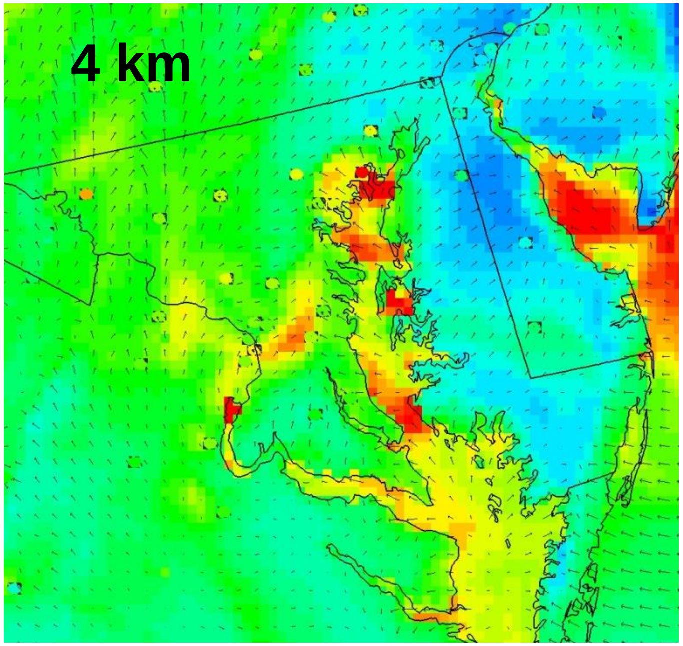
Enhancement due to feedback at locations where $[O_3] > 75$ppb

Reduction in PBL heights results in increased O_3

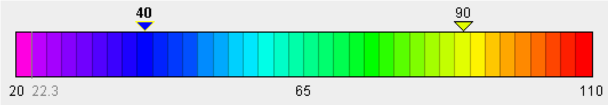
➡ **Feedback effects could have important air quality impacts**

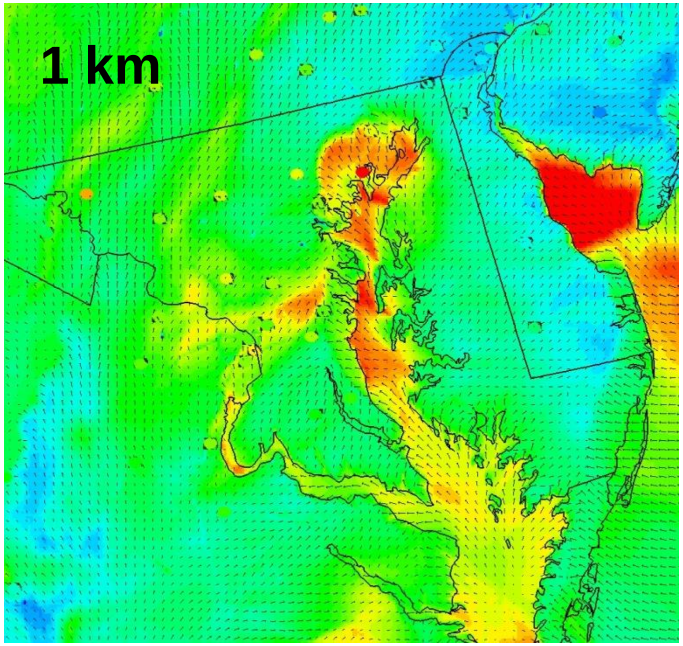
Emerging need: Improvements in Fine-scale simulations





O_3 at 3pm LT



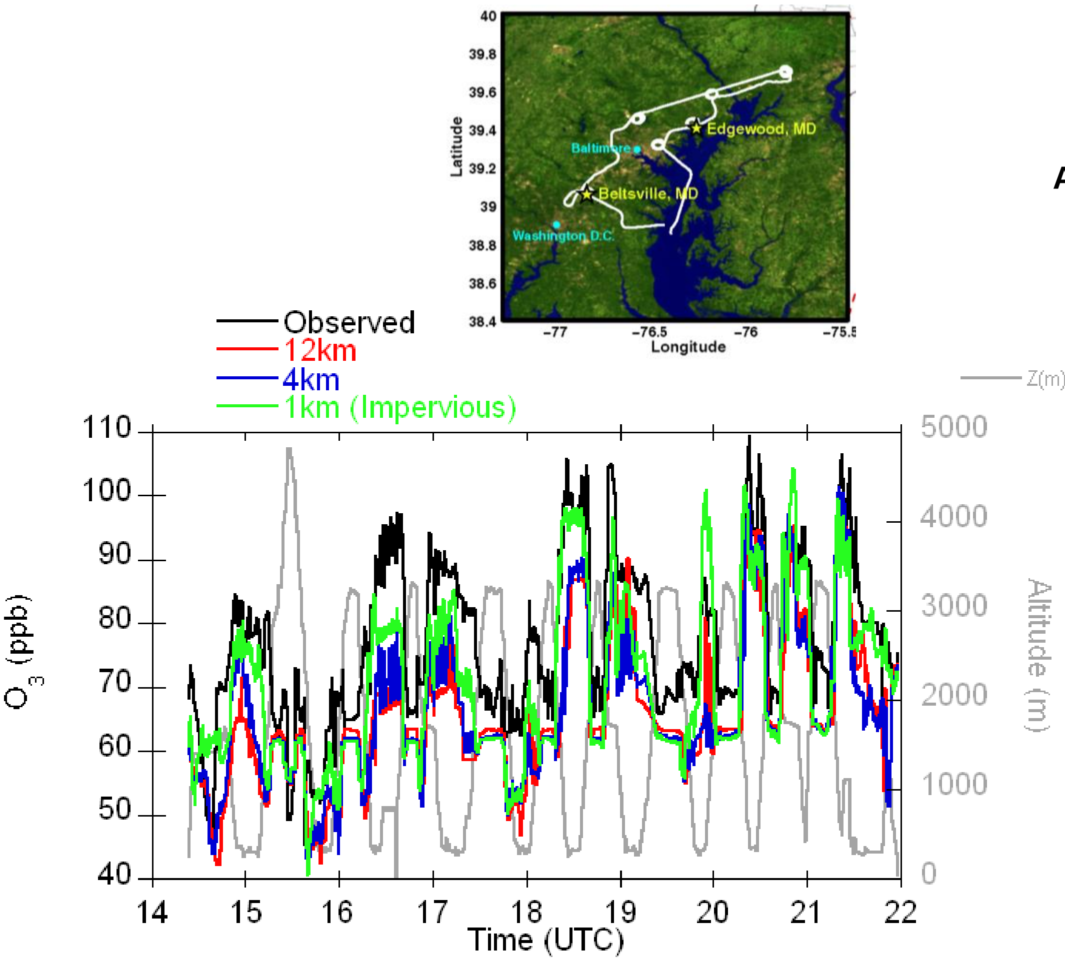


Representing spatial gradients

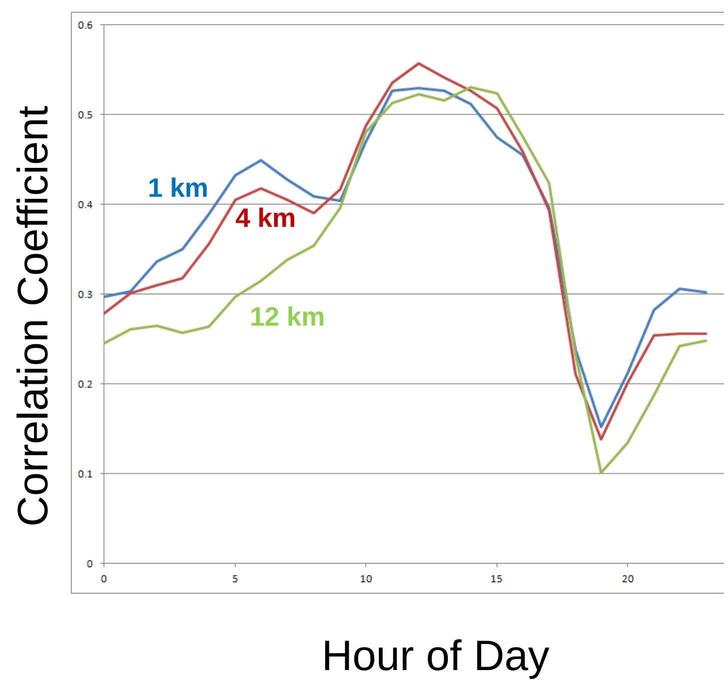
- Bay breeze impacts on inland monitors

Improvements in Fine scale simulations

Comparison with aircraft measurements
DISCOVER-AQ; July 2, 2011

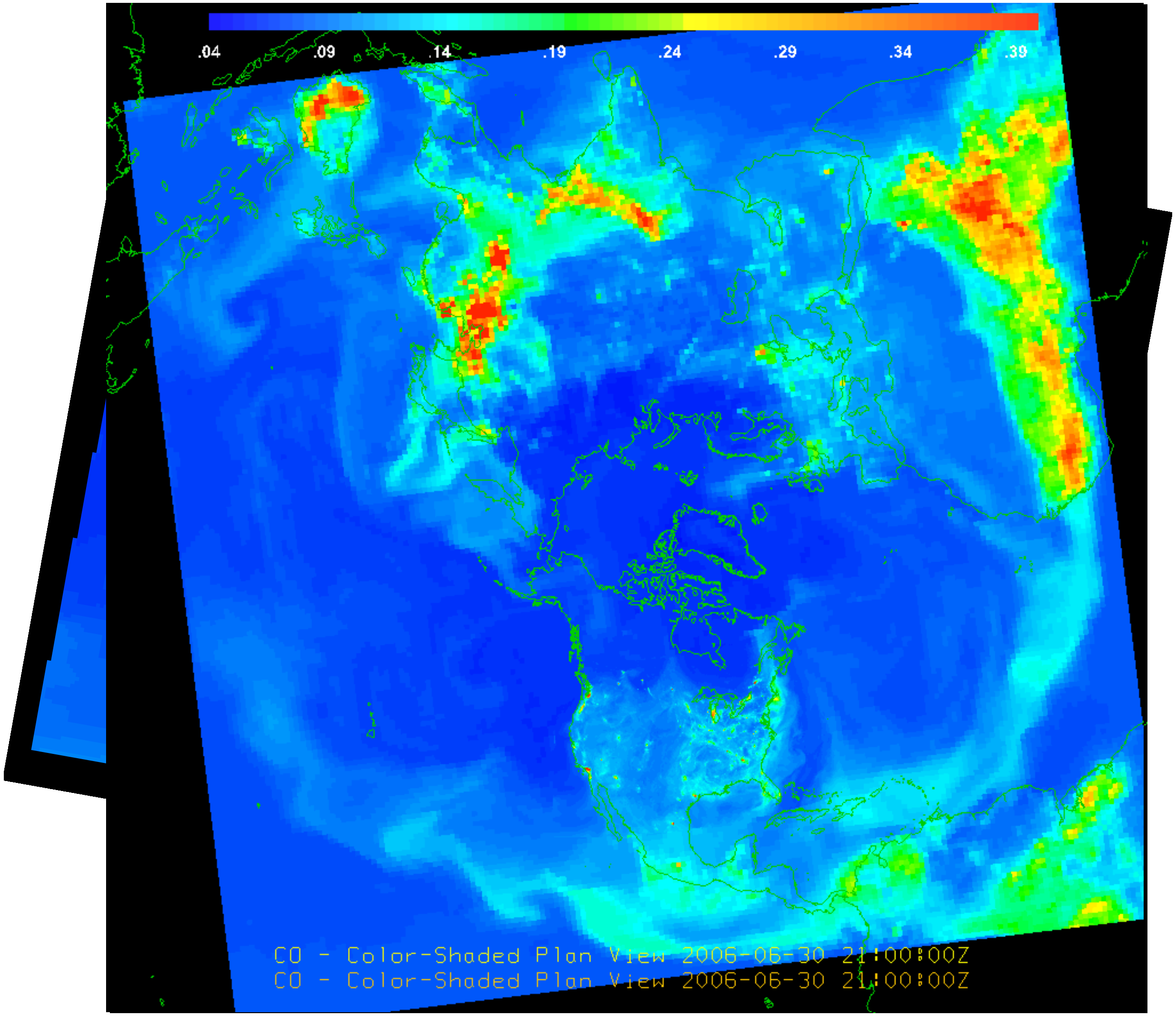


Average Diurnal Cycle of Obs/Mod Correlations (R^2) Across Space for 69 AQS O3 Monitors



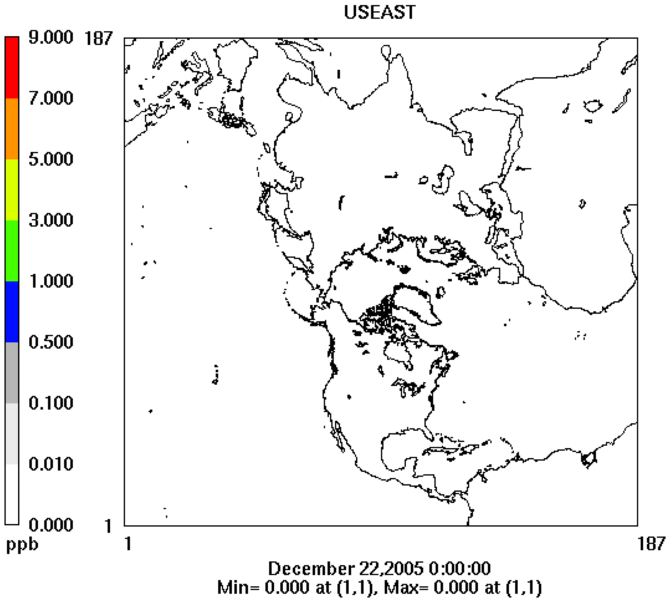
Traditional CMAQ Applications: Regional-scale

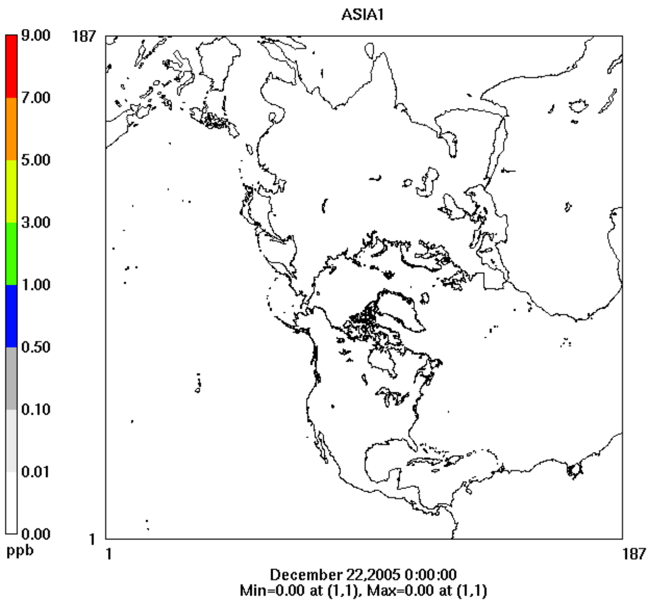
Emerging Need: Examining U.S. air quality in context of the global atmosphere



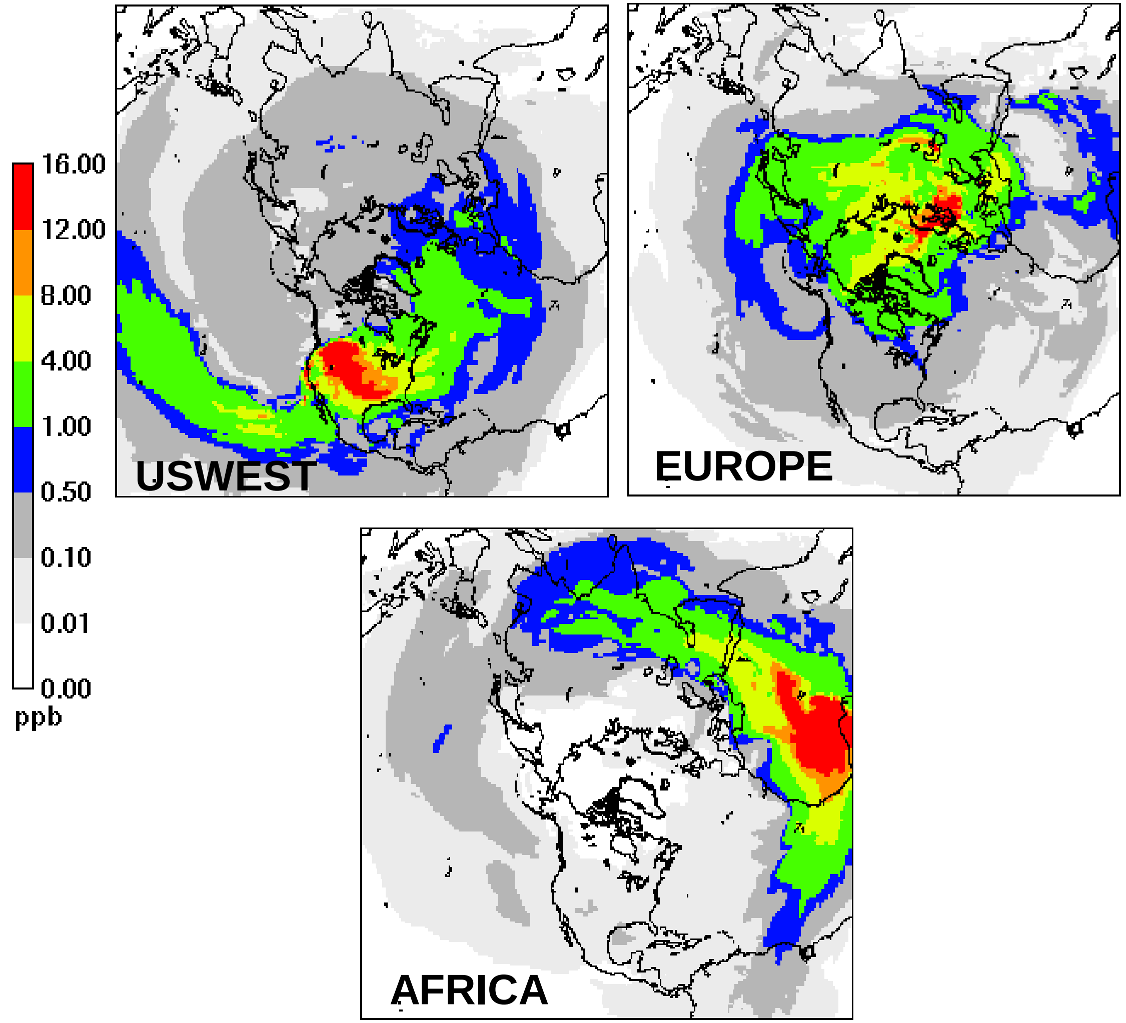
Tracer Transport: 12/22/05-1/20/06 Layer 22 (2.6-3.2km)

Tracers emission: 200 moles/s over 5x5 grid cells at the surface
USWest, USEast, Asia1, Asia2, Africa, Europe



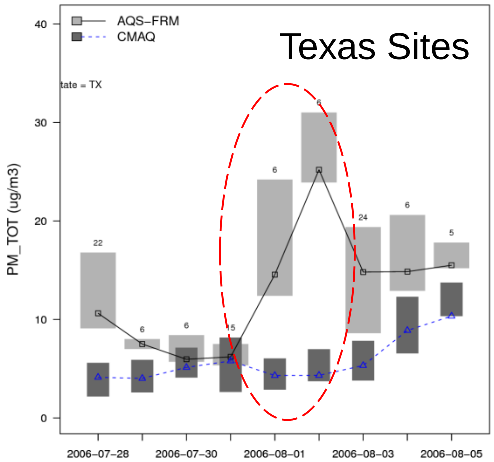


Tracer Footprint: Maximum values



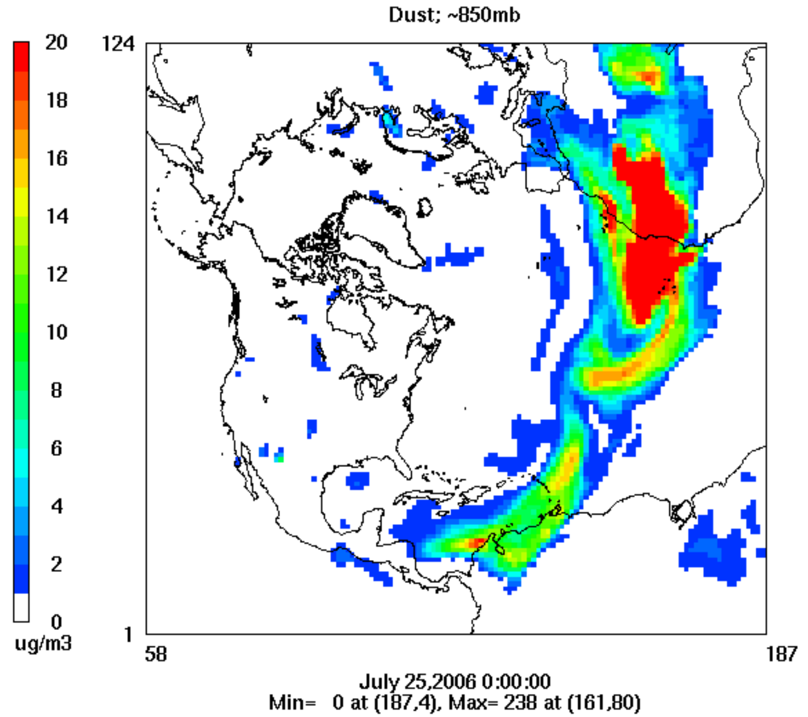
Representing Impacts of Long-Range Transport

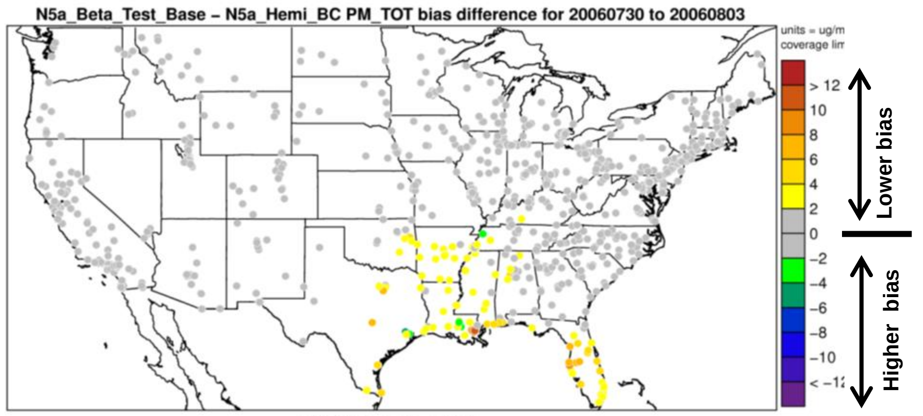
Transport of Saharan Dust: Summer 2006



Surface PM concentration in the Gulf states impacted by LRT during July 30-Aug 3

Dust Transport: 850 mb

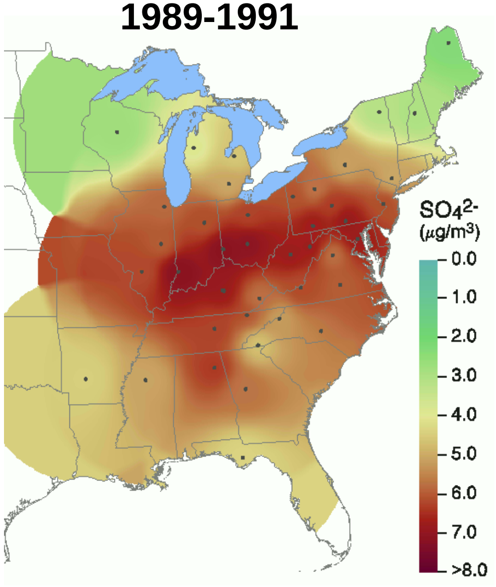




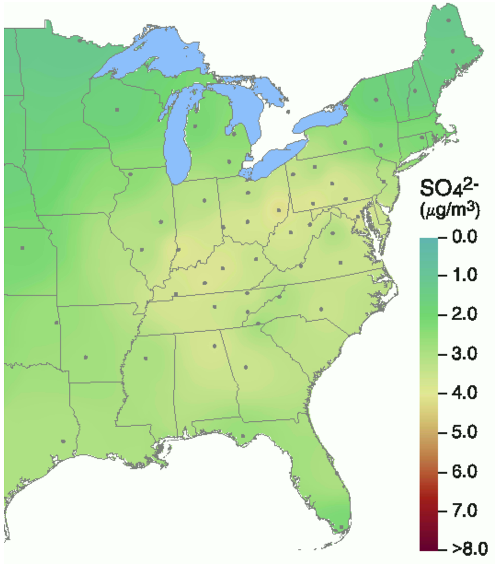
New Directions: Testing/Evaluating Aerosol Radiation Effects

Can models capture past trends in aerosol loading and associated radiative effects?

1989-1991



2007-2009

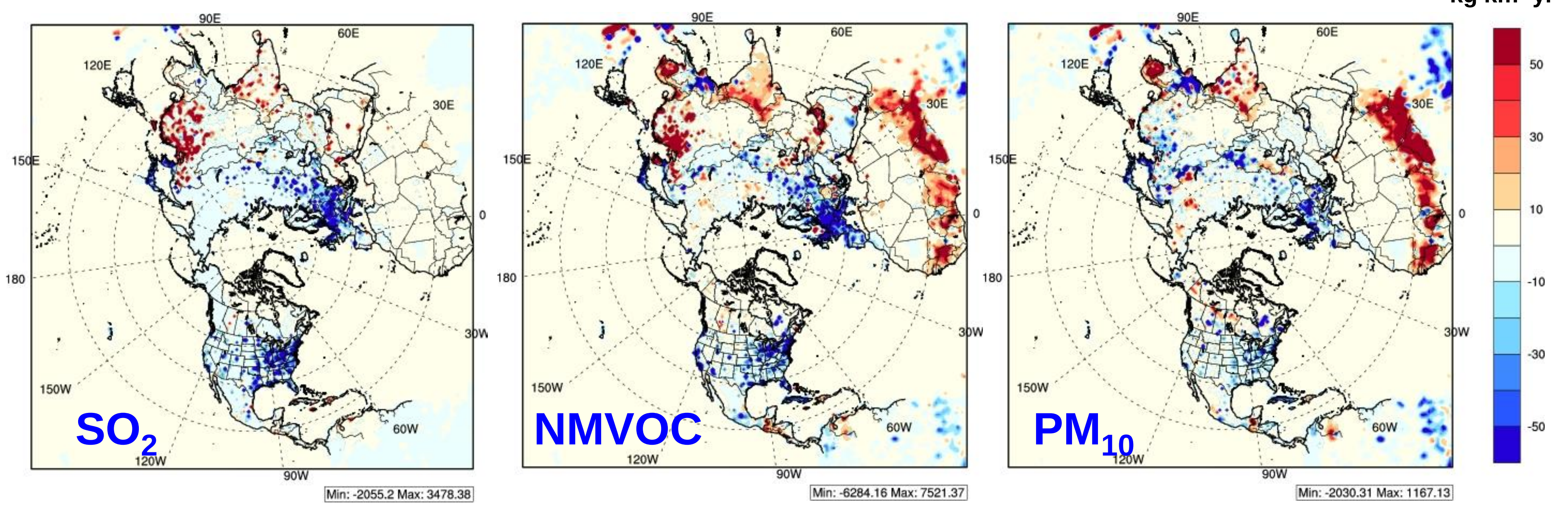


USEPA/CAMD

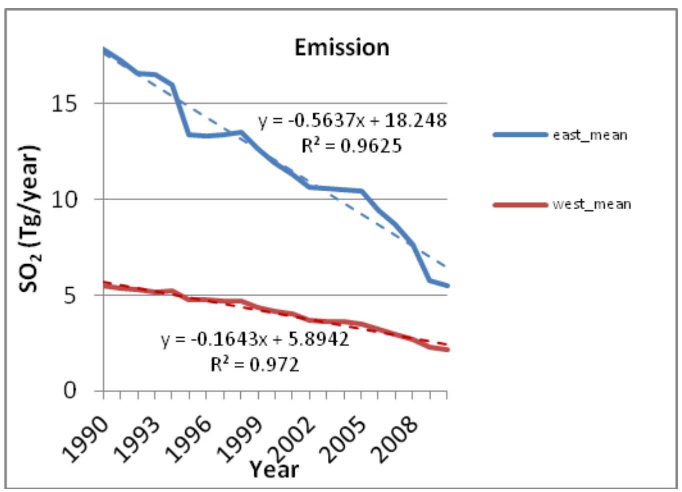
- Title IV of the CAA achieved significant reductions in SO_2 and NO_x emissions from EGUs since the 1980s
- Tropospheric SO_4^{2-} burden has reduced significantly
- Can the associated increase in surface solar radiation be detected in the measurements and models ("*brightening effect*")
- Multi-year WRF-CMAQ simulations to assess the responsiveness of the model to Title IV emission changes are now being set-up

How do changing emission patterns impact background pollution levels?

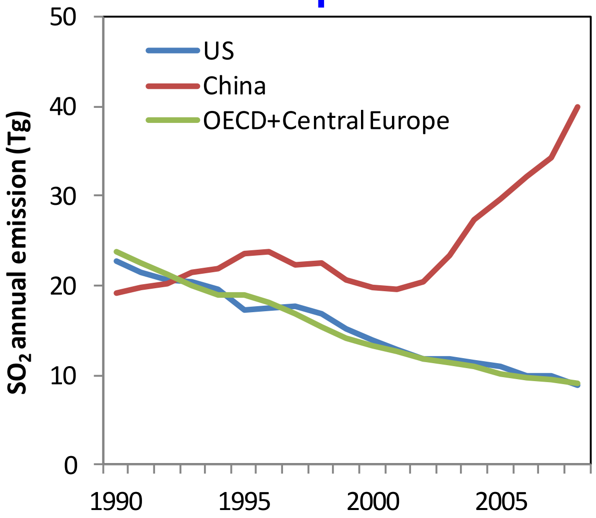
Multi-decadal (1990-2010) Trends In Emissions



U.S. Emission Trends



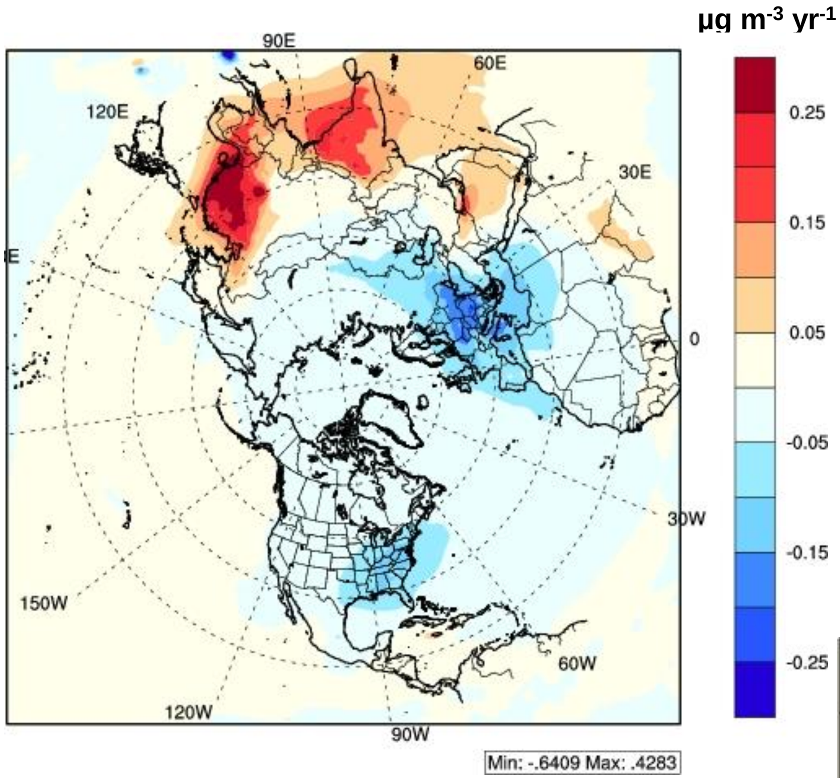
Northern Hemisphere Emission Trends



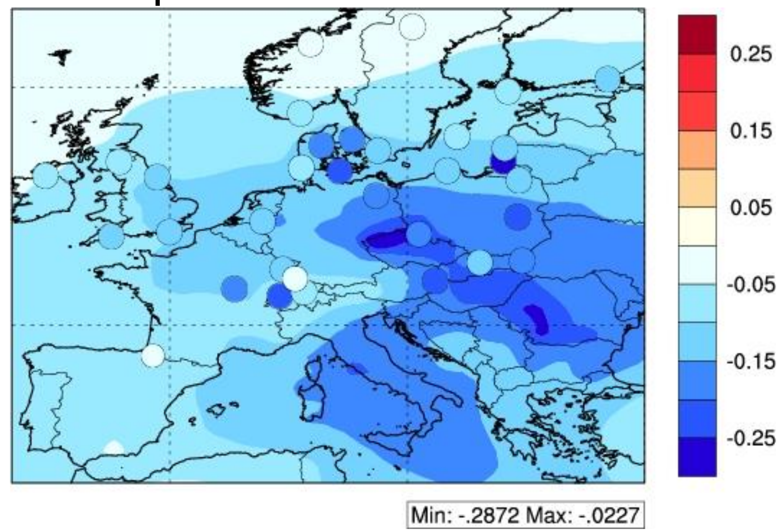
Simulated and Observed 1990-2010 Trends

Annual mean SO_4^{2-}

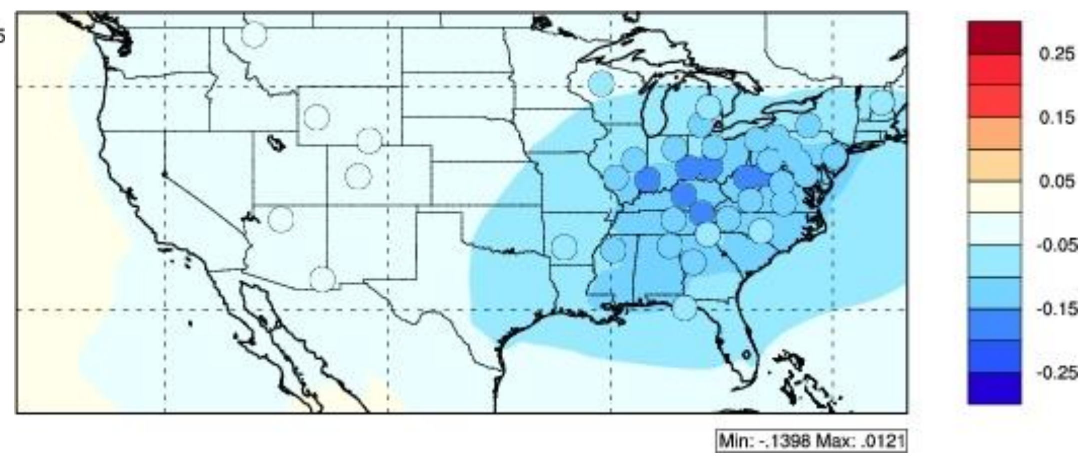
United States Environmental Protection Agency



Comparison with EMEP

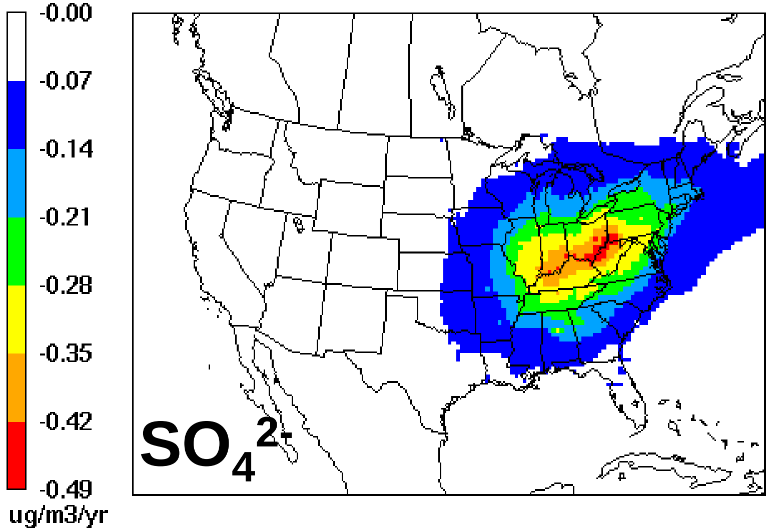


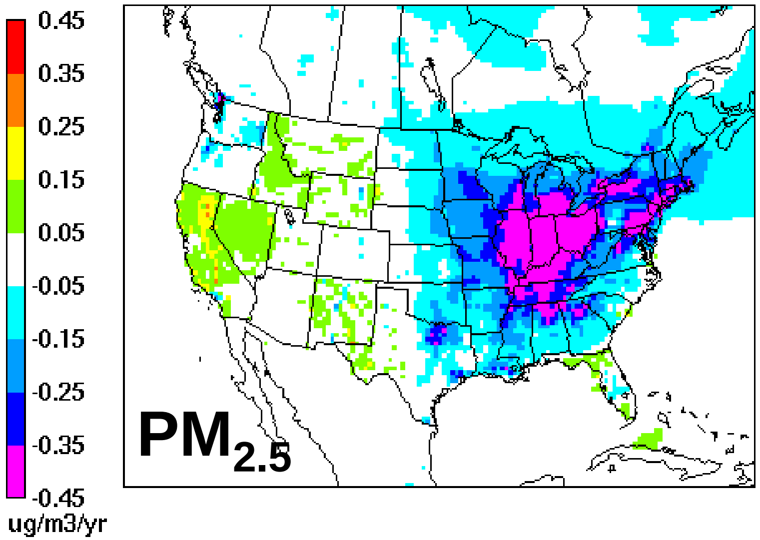
Comparison with CASTNET



Simulated and Observed 1990-2010 Trends

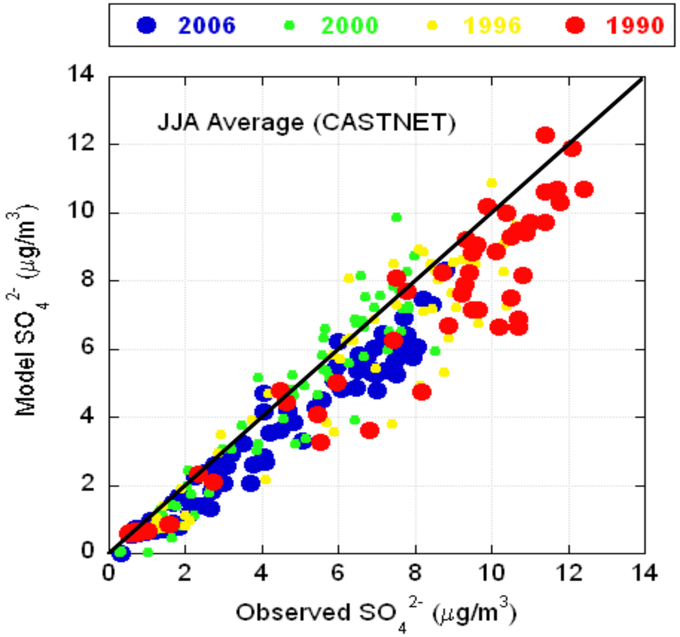
Summer mean tropospheric aerosols (SO_4^{2-} & $PM_{2.5}$)





Large reductions in surface $PM_{2.5}$ in East US

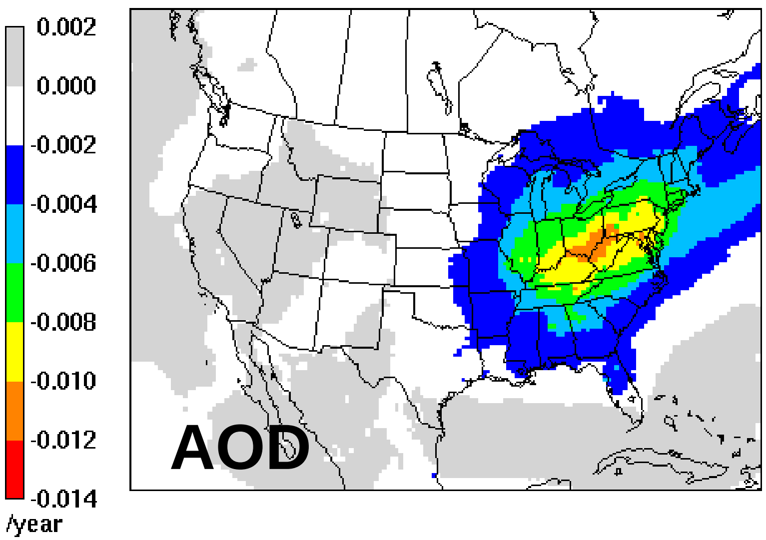
Changes in observed SO_4^{2-} captured by the model

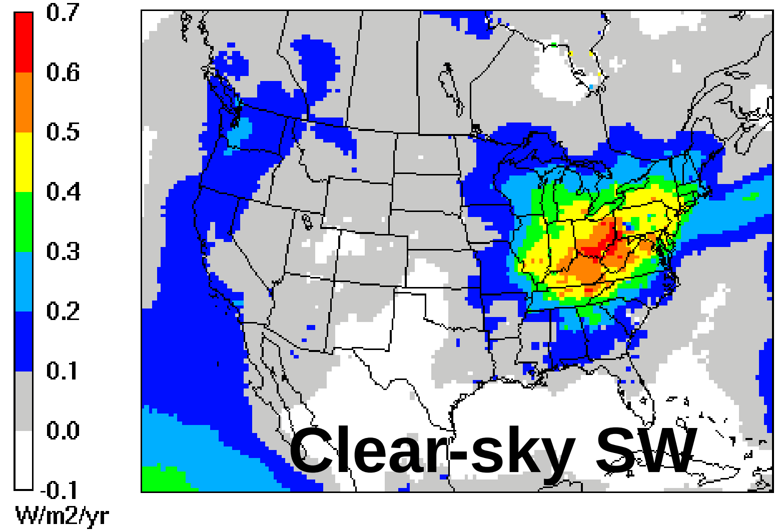


Office of Research and Development
Atmospheric Modeling & Analysis Division
National Exposure Research Laboratory

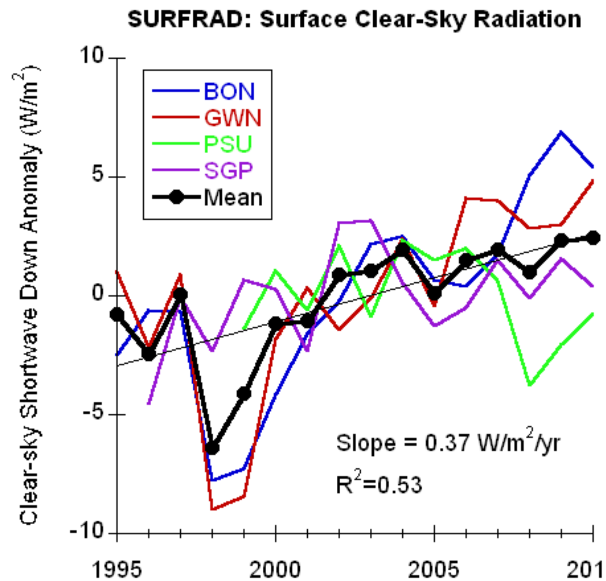
Simulated and Observed 1990-2010 Trends

Tropospheric aerosols Optical & Radiative Properties



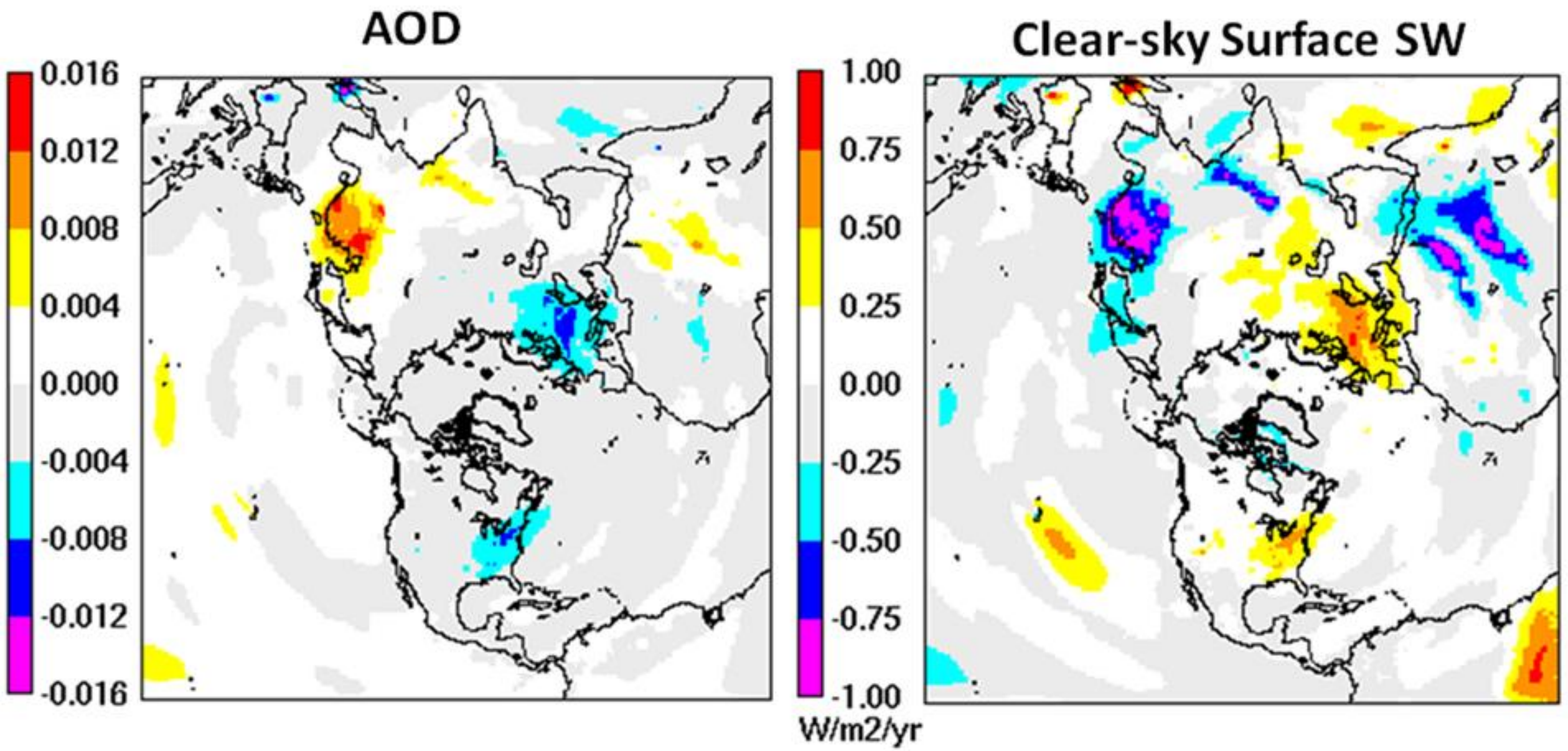


- Significant reductions in tropospheric aerosols in East US resulting from emissions reductions
- Some increase in background
- Radiation brightening in regions where aerosol burden has reduced
- Magnitude of model estimated brightening similar to that inferred from measurements in East US



Simulated and Observed 1990-2010 Trends

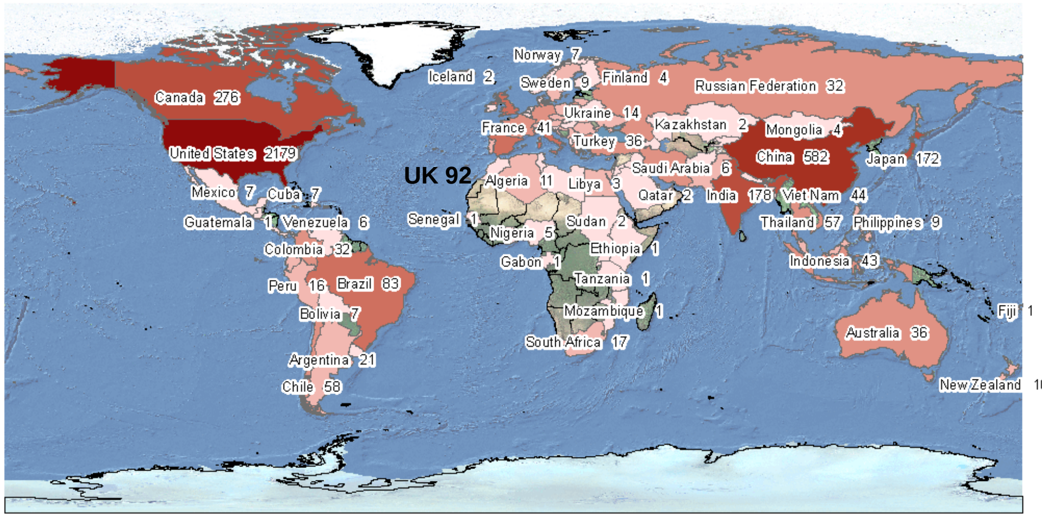
Spatial Heterogeneity in Aerosol Optical & Radiative Properties

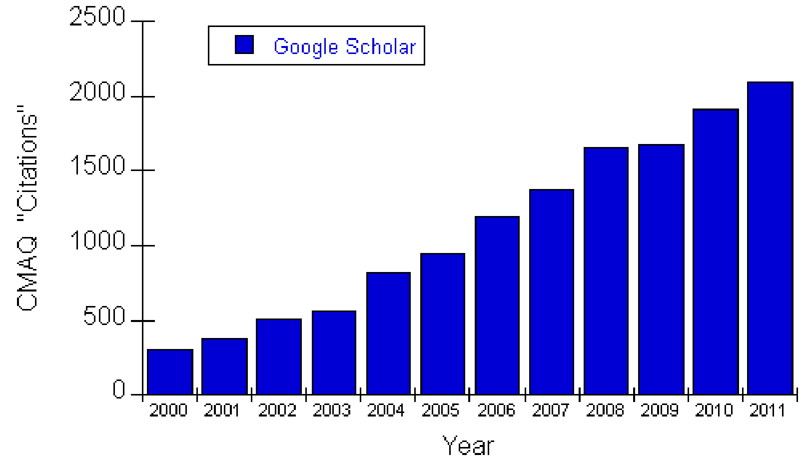


Interactions between air pollution and regional climate

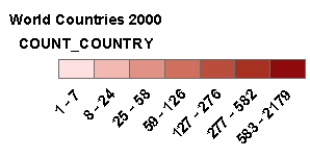
- Radiation “brightening” in North America and Europe
- Radiation “dimming” in Asia

CMAQ: A growing community of users and applications





CMAS Center Registered Users

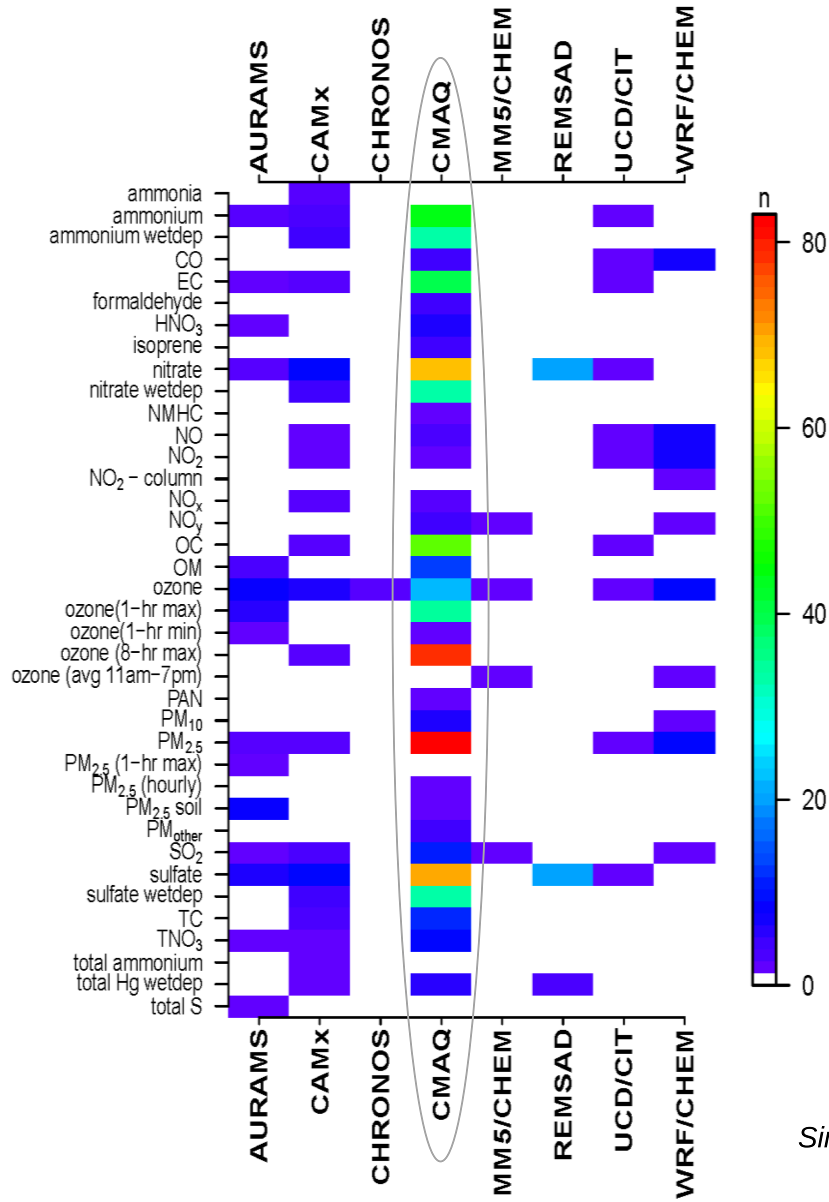


Periodic scientific updates to the CMAQ model have led to the creation of :

- **dynamic and diverse user community**
- **more robust modeling system**

CMAQ

Growing number of model evaluation studies



Simon et al., Atmos. Env. 2012

United States Environmental Protection Agency

❑ Summary

– CMAQ has evolved considerably (processes, species, space & time scales, user & development community) over the past decade to address the increasingly complex applications needed to understand and characterize emerging environmental issues

❑ Acknowledgements

– Numerous scientists in the Atmospheric Modeling and Analysis Division, U.S. EPA have contributed to the development, evaluation, and evolution of the CMAQ modeling system

❑ Model code and documentation available at:

– http://www.cmascenter.org/