United States Environmental Protection Agency

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

Past, Recent Developments, and New Directions

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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

Evolution of Air Quality Models

To address increasingly complex applications and assessments

Regulatory & Assessment Needs

1970	1977	1980	1990	1994	1997	2000	2004	2008	2010	2016+
CAA -Standards -Assessments	CAAA -PSD -New Source Permitting	NAPAP	CAAA	1-hr O3 SIP	NAAQS 8-hr O_3 PM 2.5	NATA & Air Quality Forecasting		SIPs Due - 8-hr O_3 -PM - Hg -Toxics	Climate & Air Quality Interactions Exposure	Lower NAAQS
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

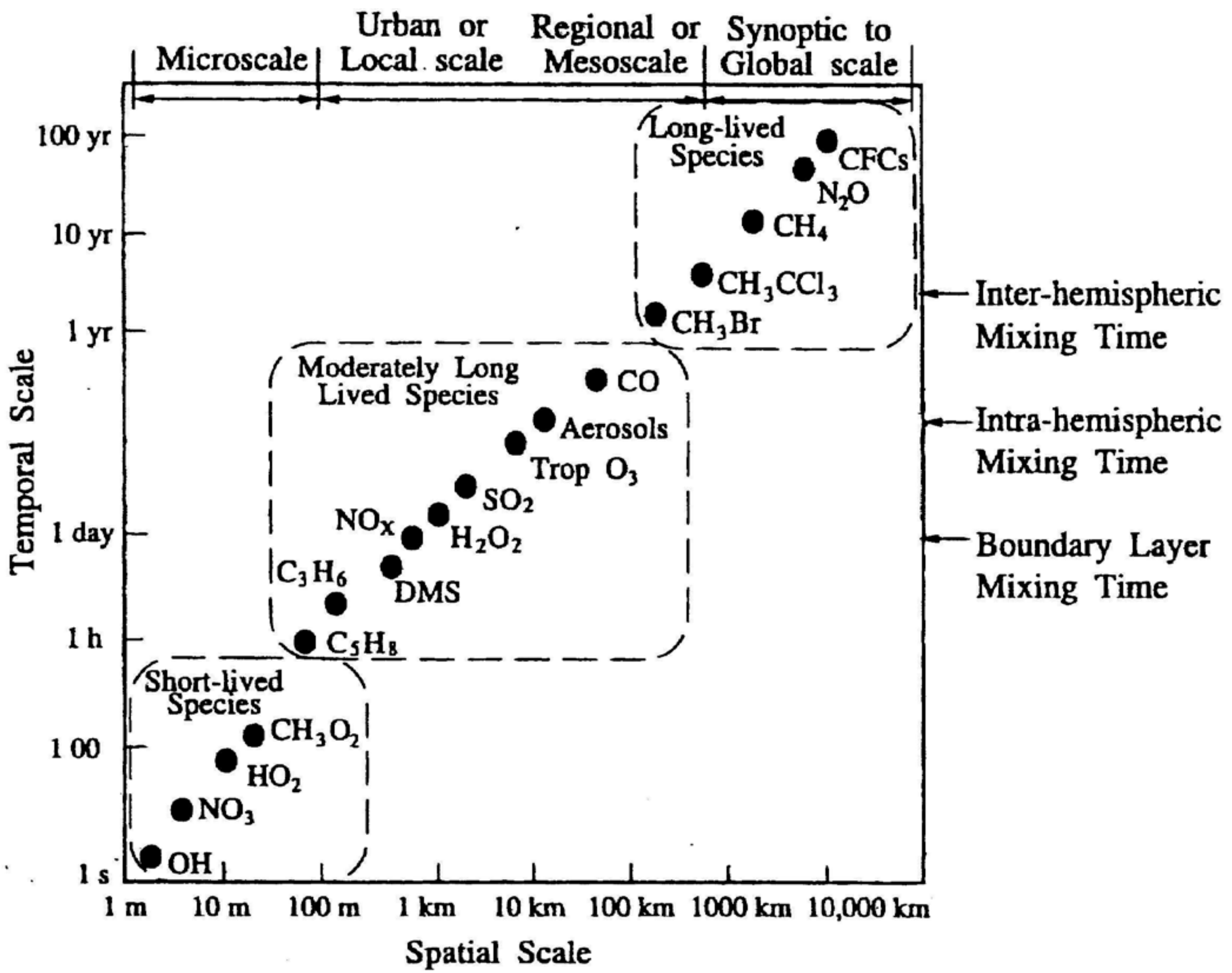
Multi-pollutant
Multi-scale (***local to hemispheric***)
Interactions with Climate forcing and Air Quality changes
Reactive
Eulerian Grid

**Atmosphere-Biosphere
Multi-scale (local to global)**

Model Development & Application

Atmospheric Pollutants

Space and Time-scales



Adapted from Seinfeld and Pandis

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

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

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

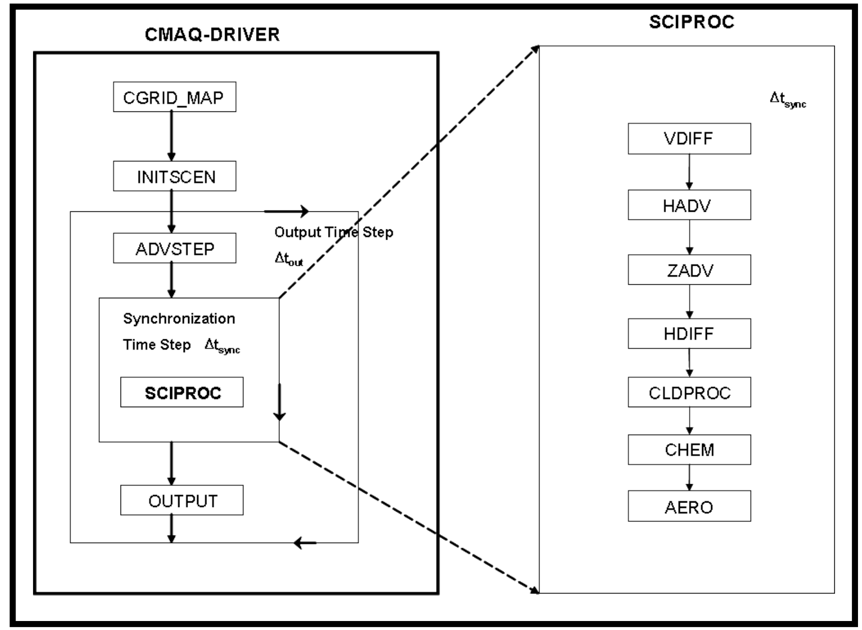
$$= \sqrt{\hat{\gamma}}\, R_{\varphi_i}(\overline{\varphi}_1,\ldots,\overline{\varphi}_N) + \sqrt{\hat{\gamma}}\, S_{\varphi_i} + \left.\frac{\partial(\varphi_i^*)}{\partial t}\right|_{cld} + \left.\frac{\partial(\varphi_i^*)}{\partial t}\right|_{aero}$$

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



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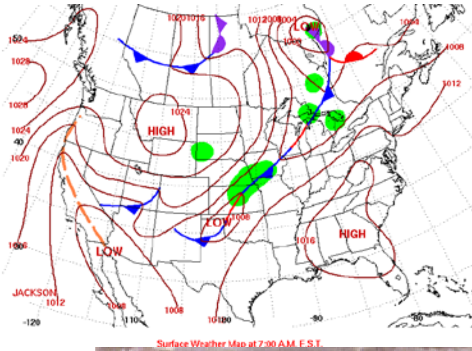
CMAQ Modeling System



Meteorological Model (WRF)

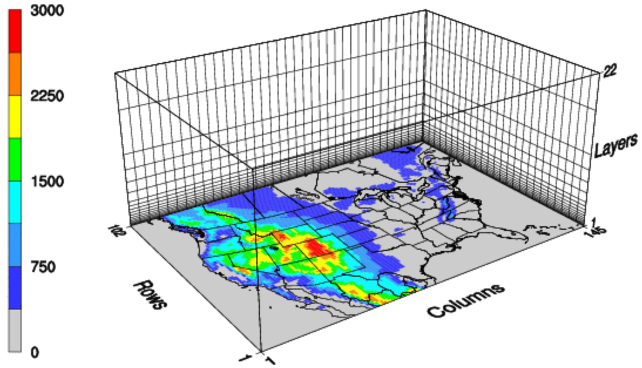
Meteorological-Chemical Interface Processor (MCIP) (AQPREP)

SMOKE

Anthropogenic and Biogenic Emissions processing

CMAQ AQ Model-

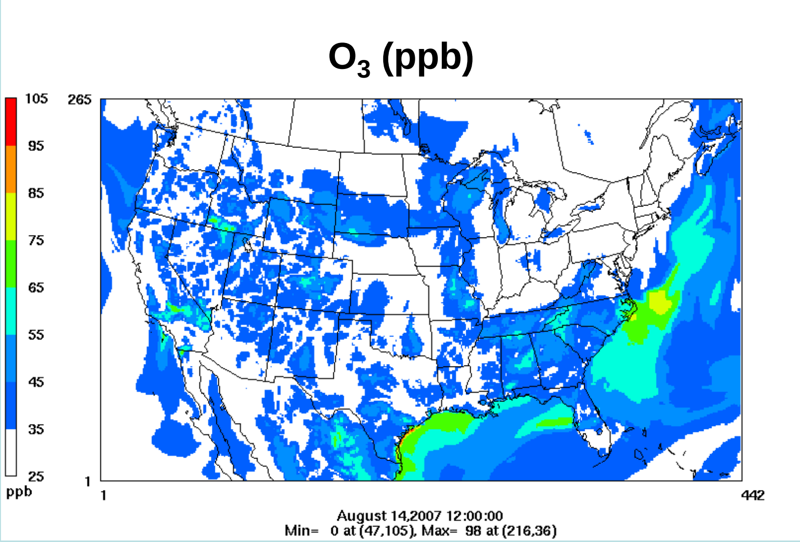
Chemical-Transport Computations



The Community Multiscale Air Quality (CMAQ) model:

- **Eulerian** grid chemical transport model
- **Multi-scale**: Hemispheric → Continental →Regional → Local
- **Multi-pollutant (and multi-phase)**:
  - **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
  - CMAQv5.1 released in December 2015

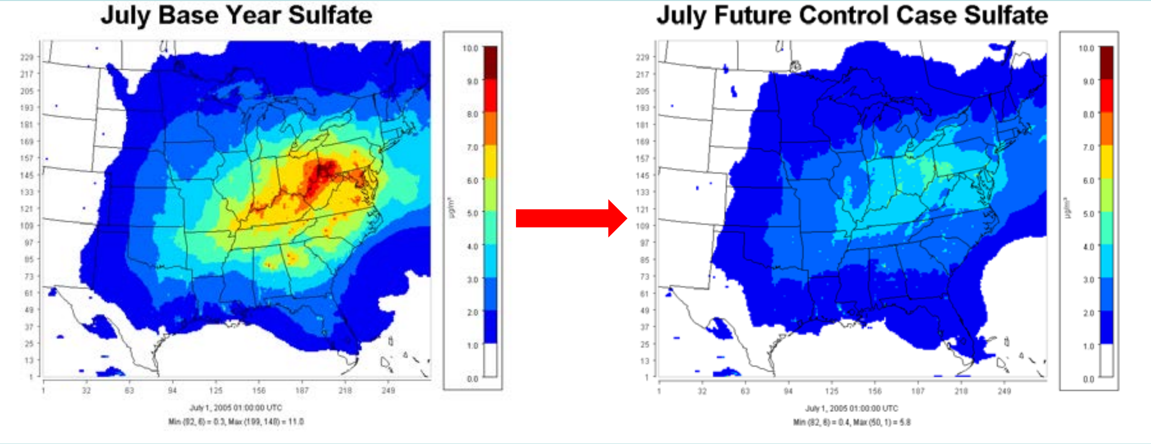
Typical Regional-Scale CMAQ Applications



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

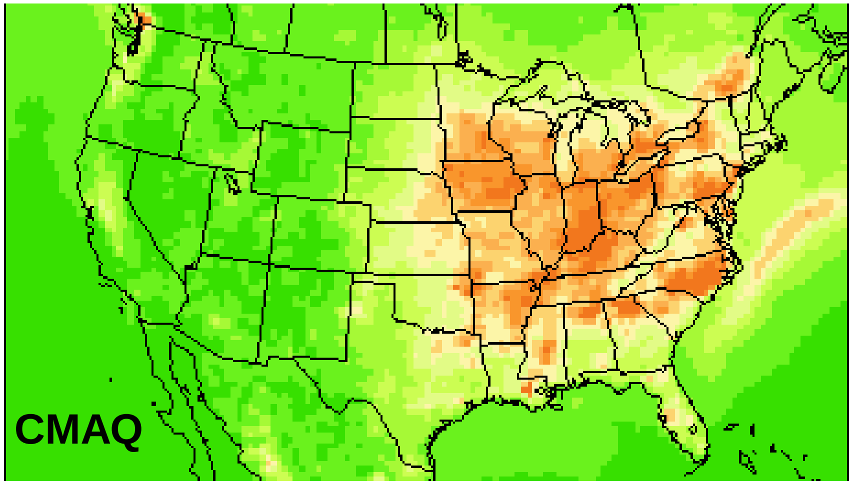
Simulating the ***effectiveness*** of emission ***control strategies***

- Clean Air Interstate Rule
- Clean Air Mercury Rule
- Renewable Fuels Standard Act-2
- State Implementation Plans

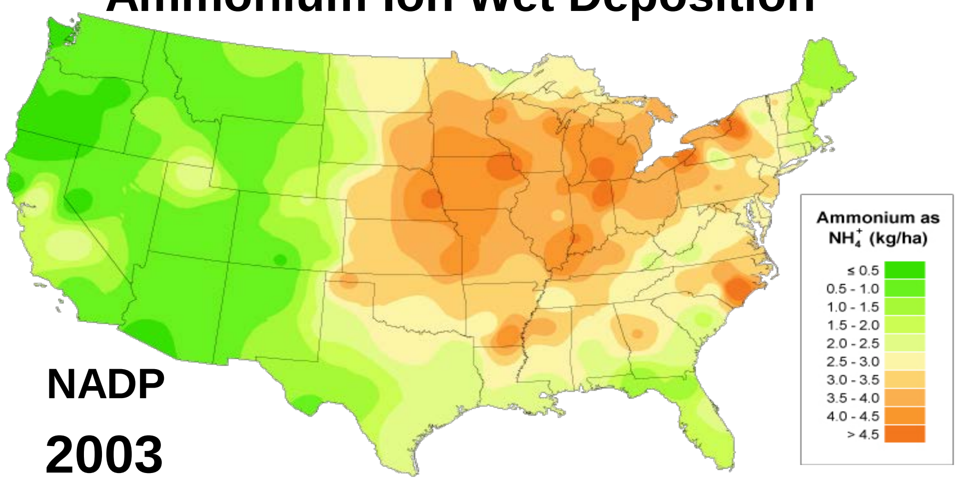


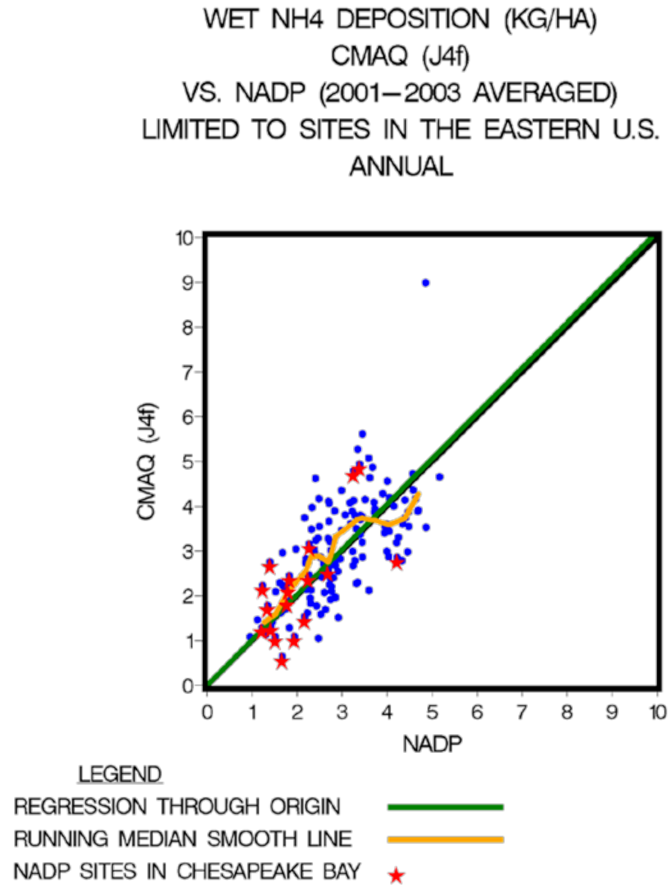
CMAQ Applications: Atmospheric N Depositions

Nutrient loading to sensitive Ecosystems



Ammonium Ion Wet Deposition



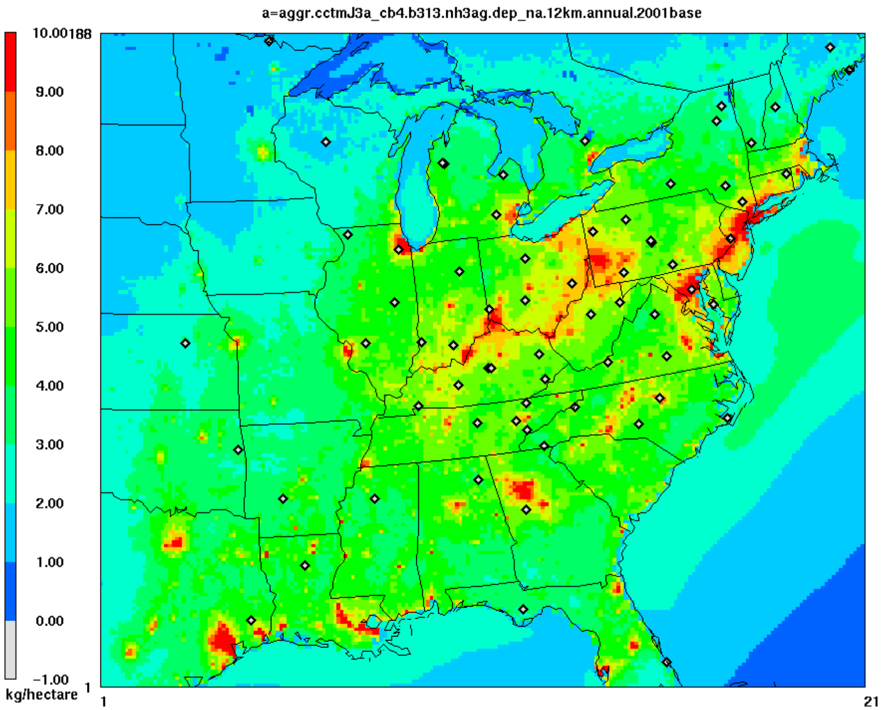


CMAQ is able to capture main spatial pattern and magnitude of wet deposition

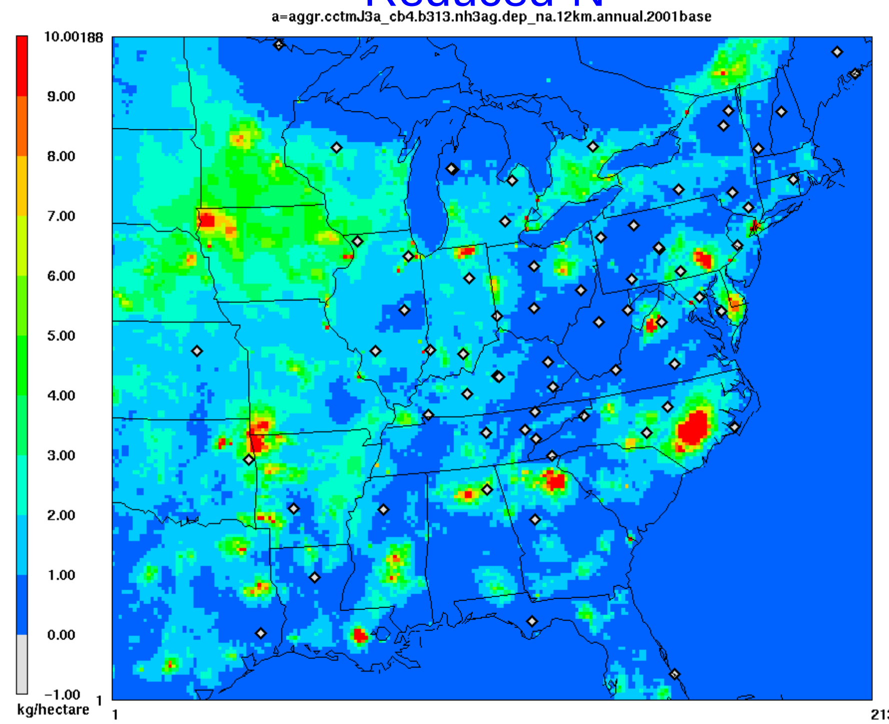
Defining Dry Deposition Monitoring Needs

Modeled spatial trends vs. CASTNET location

Oxidized-N



Reduced-N



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

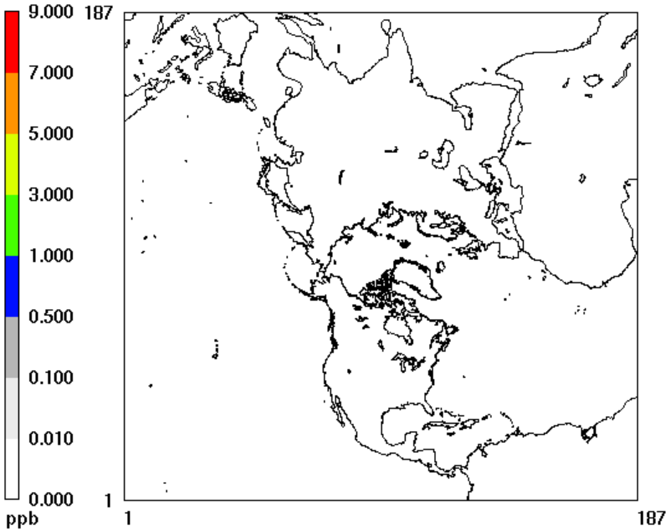
Need for greater spatial coverage

Examining U.S. Air Quality in Context of the Changing Global Atmosphere: Emerging Need

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

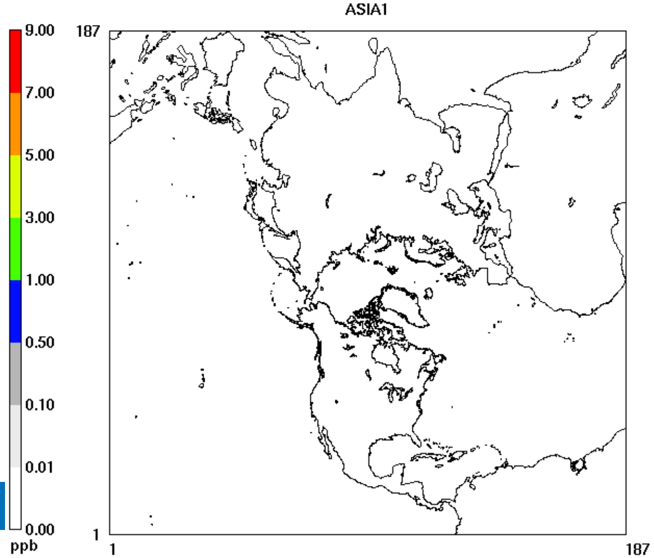
Tracers emission: 200 moles/s over 5x5 grid cells at the surface

USEAST



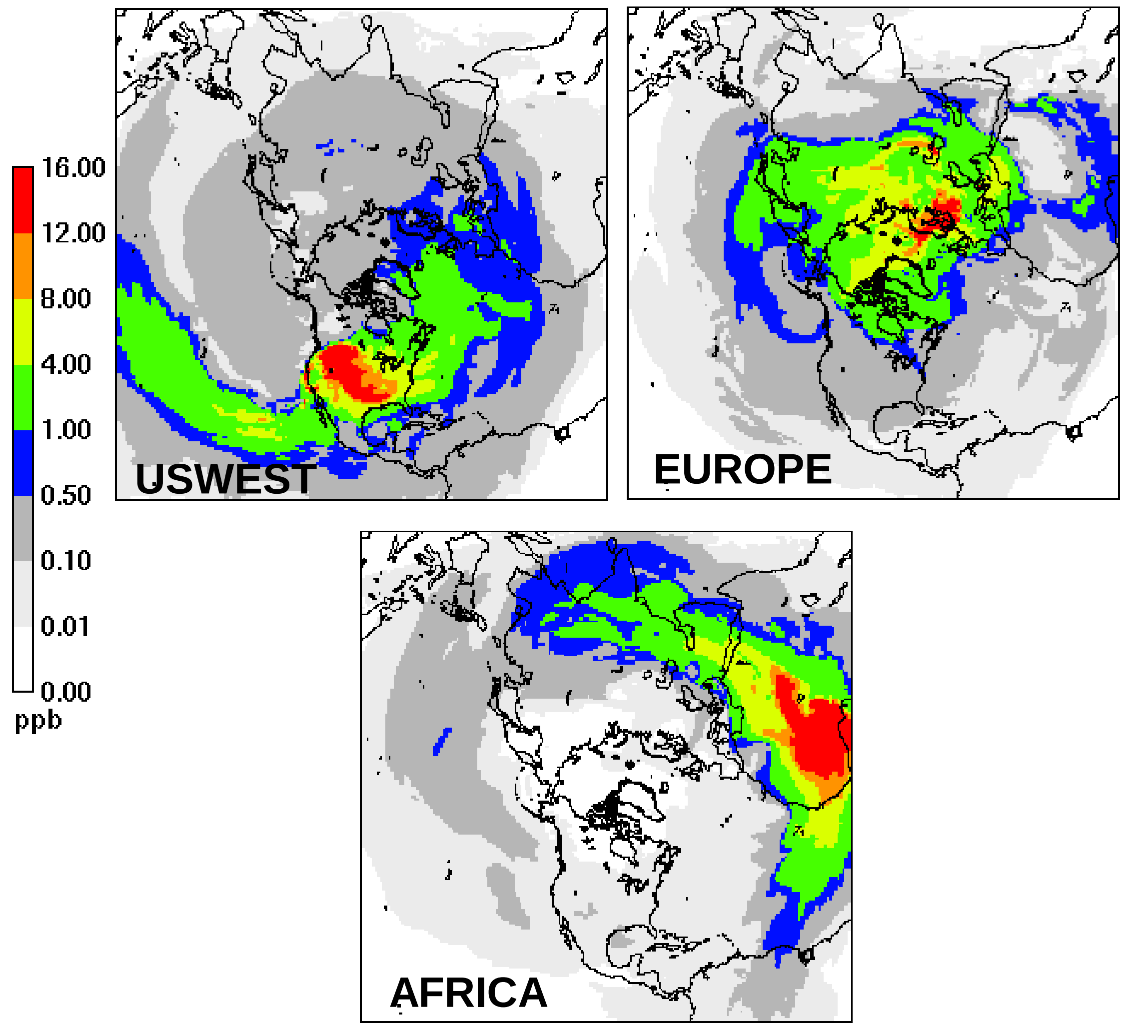
December 22,2005 0:00:00
Min= 0.000 at (1,1), Max= 0.000 at (1,1)

ASIA1



December 22,2005 0:00:00
Min=0.00 at (1,1), Max=0.00 at (1,1)

Tracer Footprint: Maximum values



Air Pollution-Radiation-Meteorology Interactions

N. Minnesota fire smoke over Chicago, 2011

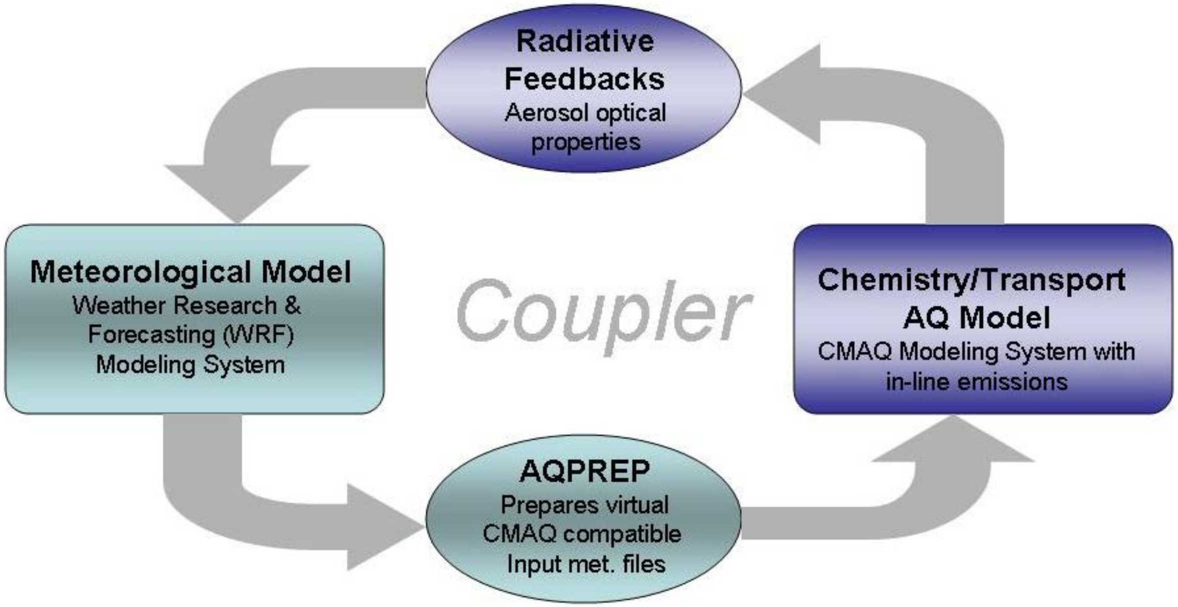
New Delhi, January 2015

AQI at U.S. Embassy: ~180-250

Phoenix, 2014: Dust Storm

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

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



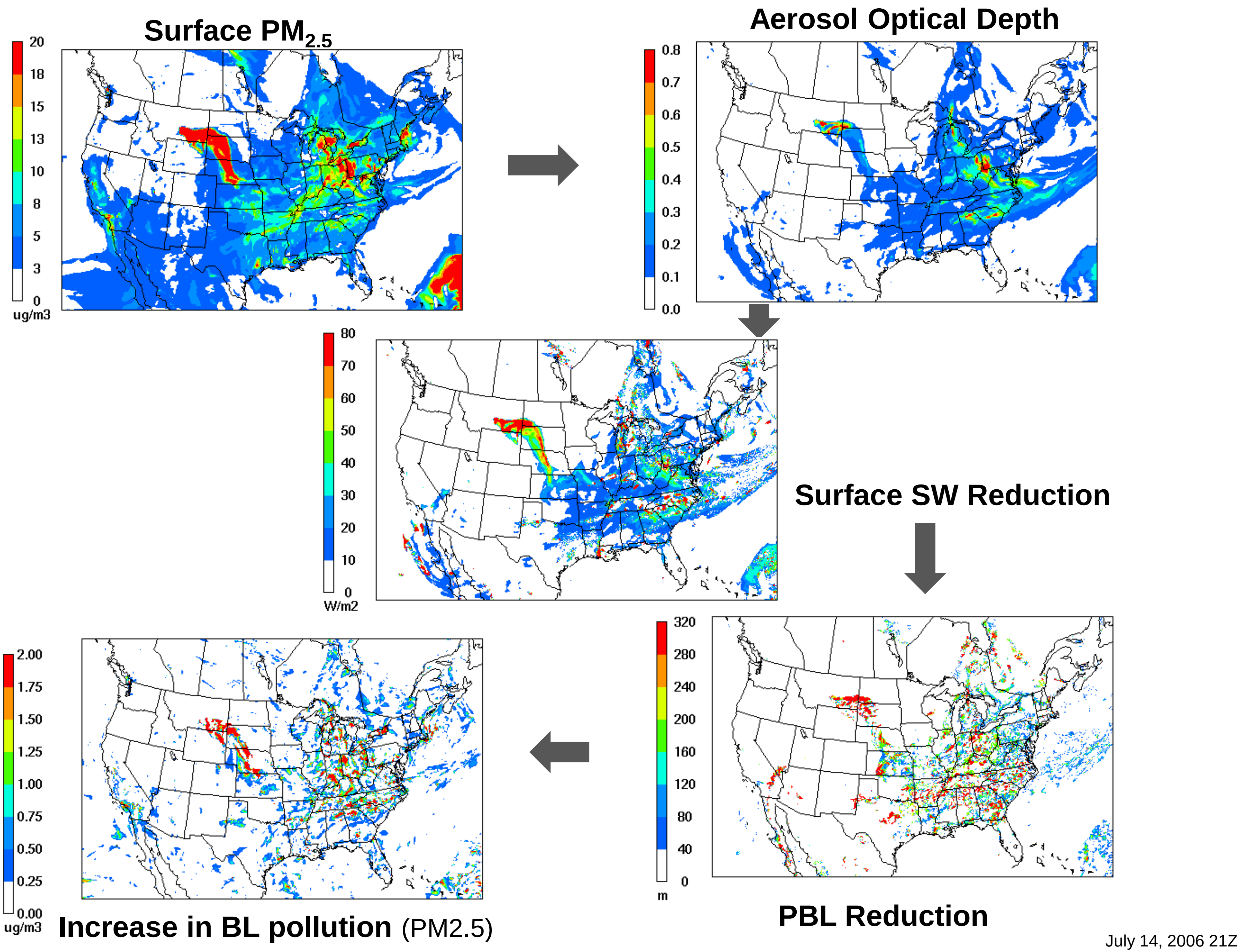
Aerosol Optics & Feedbacks

- 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**

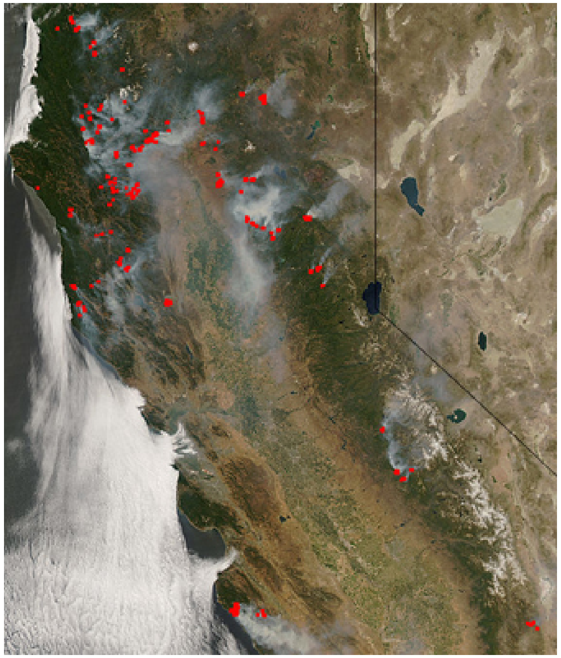
- data exchange through memory resident buffer-files
- flexibility in frequency of coupling
- identical on-line and off-line computational paradigms with minimal code changes
- both WRF and CMAQ models to evolve independently;

➡ *Maintains integrity of WRF and CMAQ*

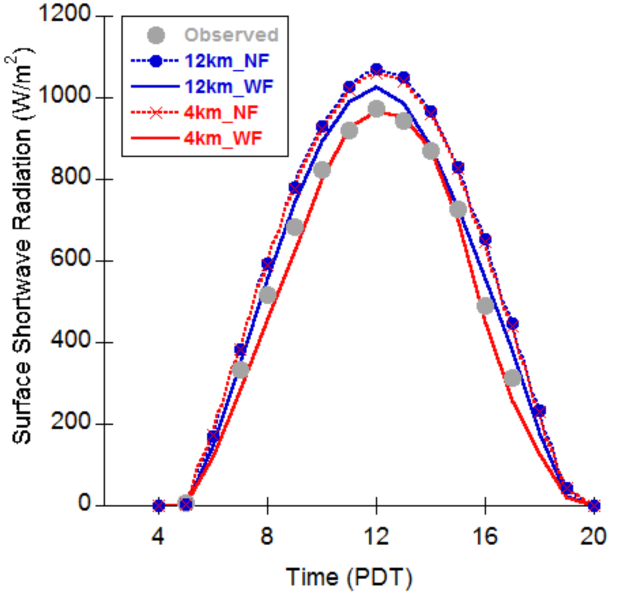

Surface $PM_{2.5}$
20
18
15
13
10
8
5
3
0
ug/m3
Aerosol Optical Depth
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
80
70
60
50
40
30
20
10
0
W/m2
Surface SW Reduction
320
280
240
200
160
120
80
40
0
m
PBL Reduction
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
ug/m3
Increase in BL pollution (PM2.5)
July 14, 2006 21Z

Case Study: California Wildfires

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



Surface shortwave radiation at Hanford

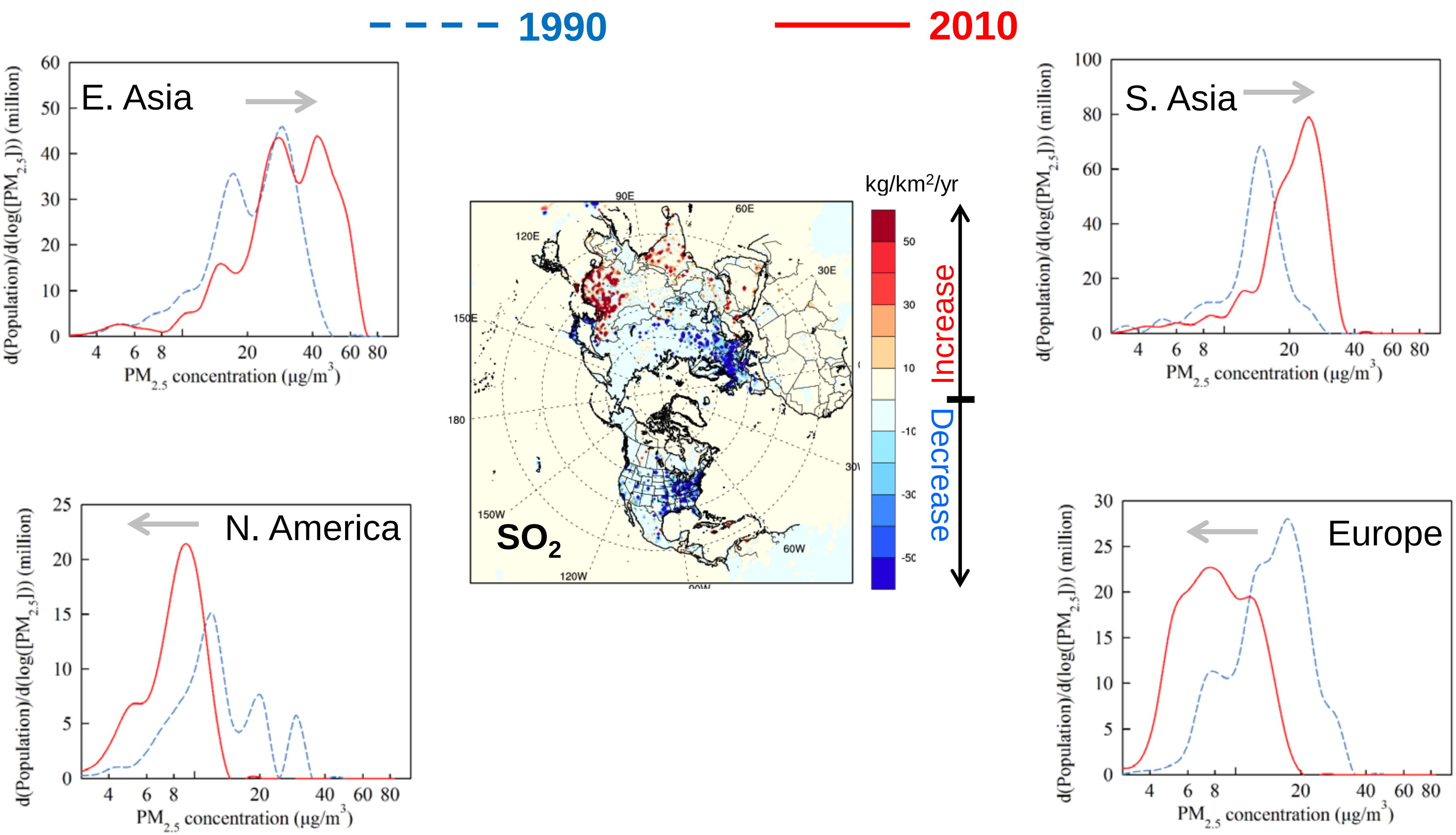


	O_3 (ppb)		$PM_{2.5}$($\mu g/m^3$)		SWR (W/m^2)		T (K)	
	NF	WF	NF	WF	NF	WF	NF	WF
ME	15.2	**14.6**	29.1	**28.6**	145.6	**112.5**	3.34	3.43
RMSE	20.2	**19.5**	48.1	**45.19**	184.2	**148.8**	4.87	**4.9**
R	0.69	0.69	0.45	**0.47**	0.86	**0.88**	0.77	**0.79**

Incorporation of feedbacks **improves performance of both meteorology and air quality** at locations impacted by smoke plumes

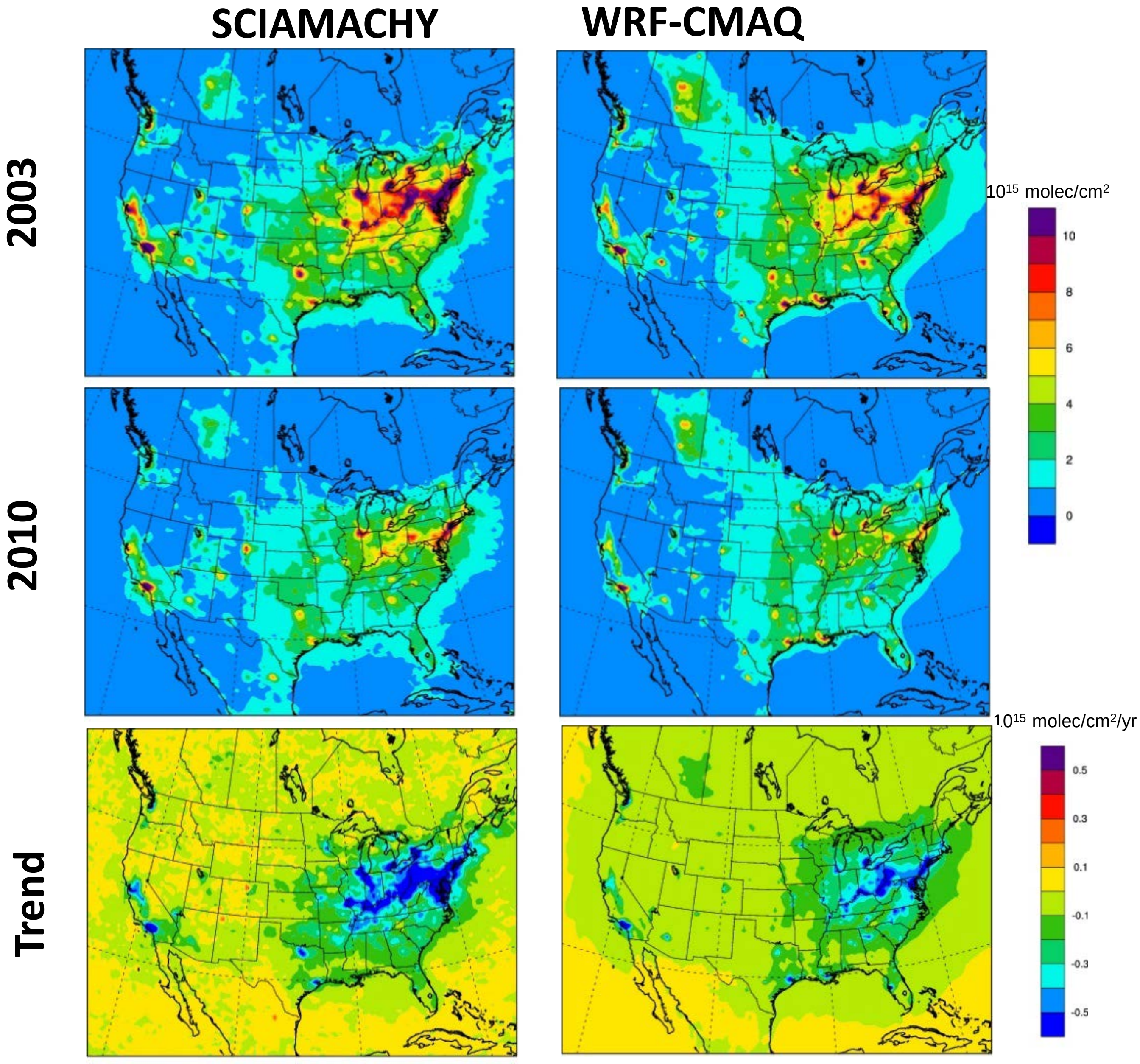
- ***Feedback effects can be important in conditions of high aerosol loading***

Need to Characterize Impacts of Changing Emissions Patterns on Air Pollution Exposure & Climate Interactions



- Contrasting changes in emissions are altering air quality on hemispheric to local scales
- In **Asia**: larger populations are being exposed to higher $PM_{2.5}$ concentrations
- **Europe/N. America**: Control measures have reduced population exposure to $PM_{2.5}$

Comparisons of Trends in NO_2 Column : 2003-2010



Both observations & model show reductions in NO_2 in urban areas and regionally

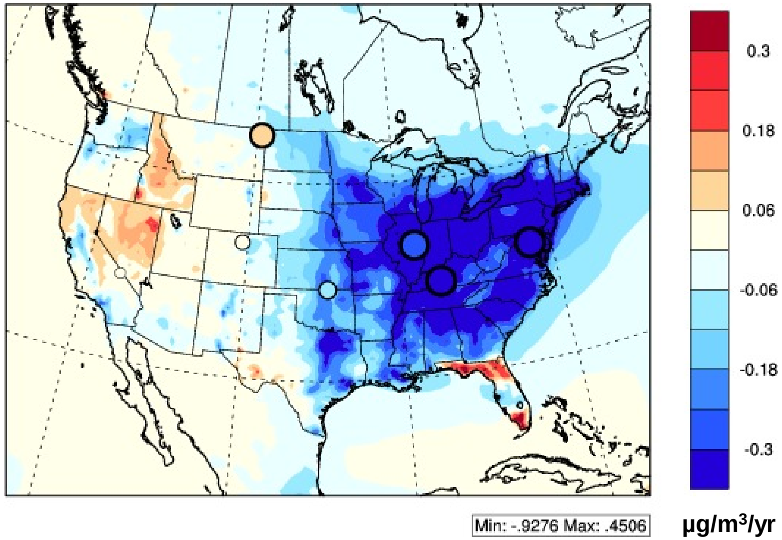
- Illustrating the impact and effectiveness of control strategies and technological advances in reducing NO_x emissions

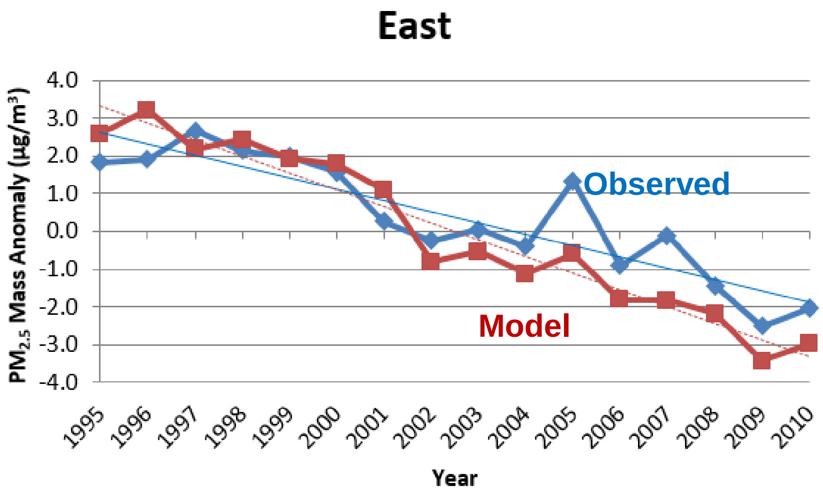
Model estimated NO_2 column as well as trend are lower than retrievals

- *What level of quantitative agreement should be expected?*

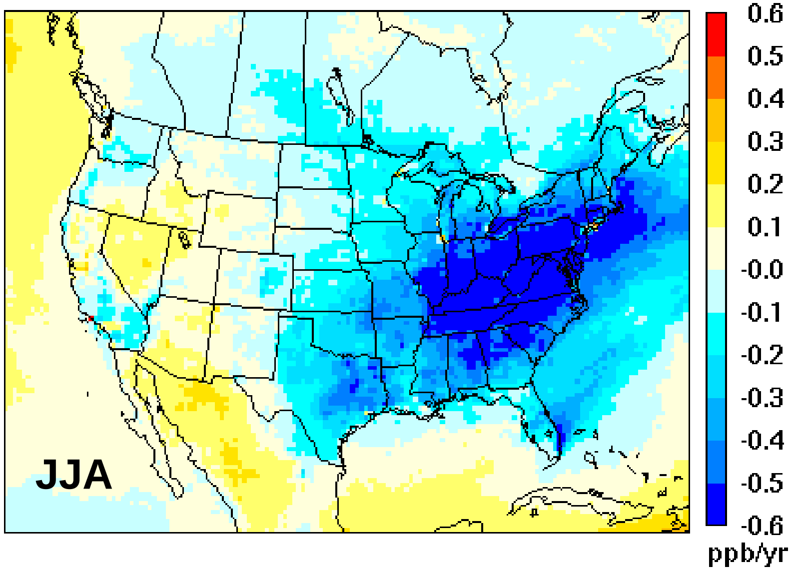
Simulated and observed Trends: 1990-2010

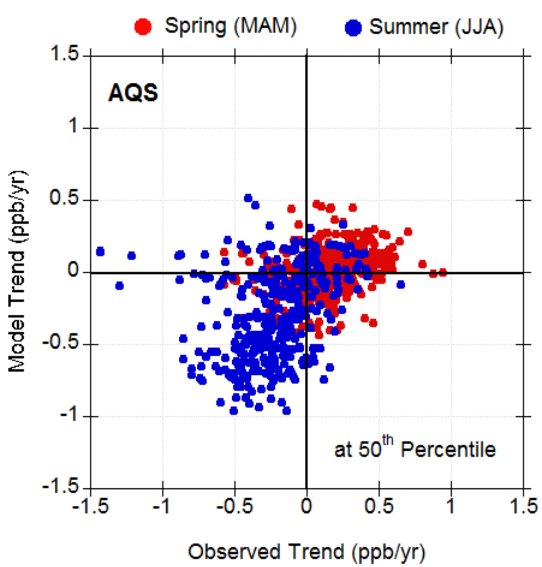
Annual $PM_{2.5}$





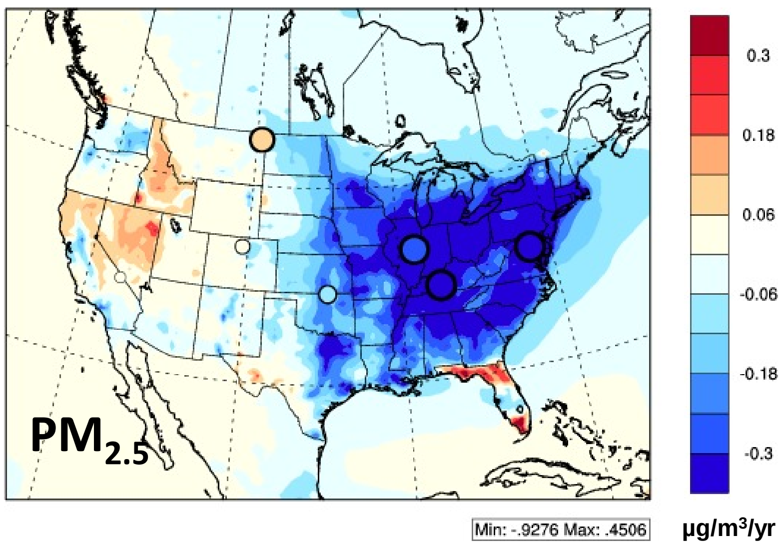
50^{th} Percentile O_3

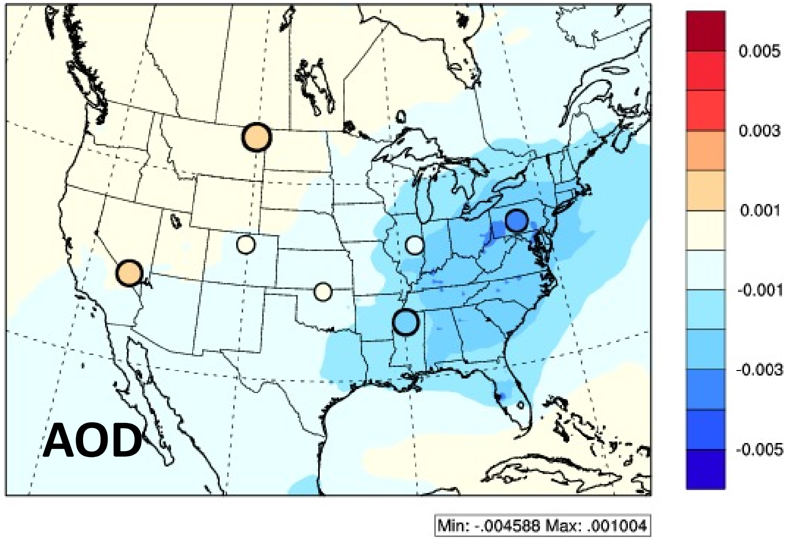


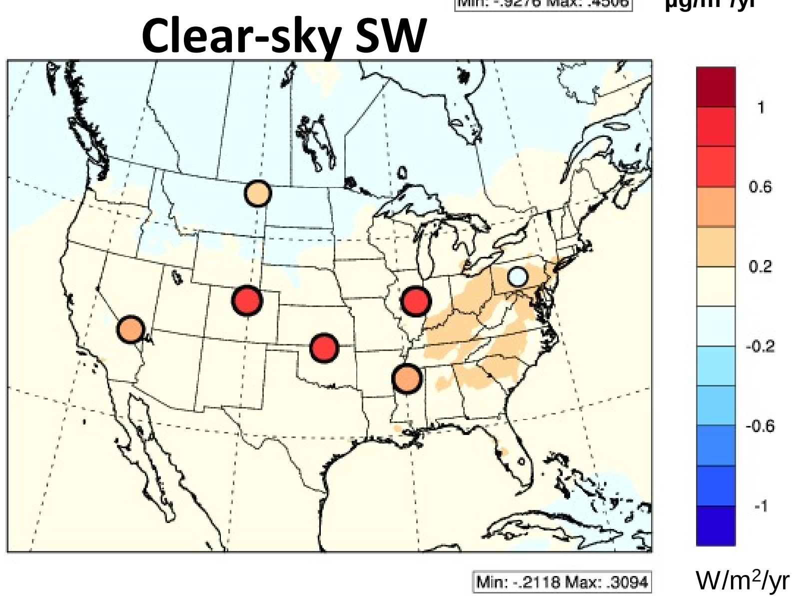


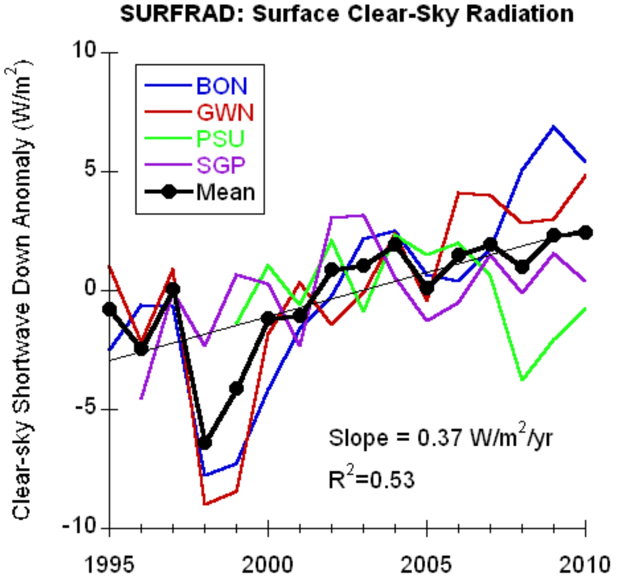
- Summer trends at the median concentration and high ranges show decreases across majority of sites
- Increasing trend at many locations during Spring

Simulated and observed Trends: 1990-2010







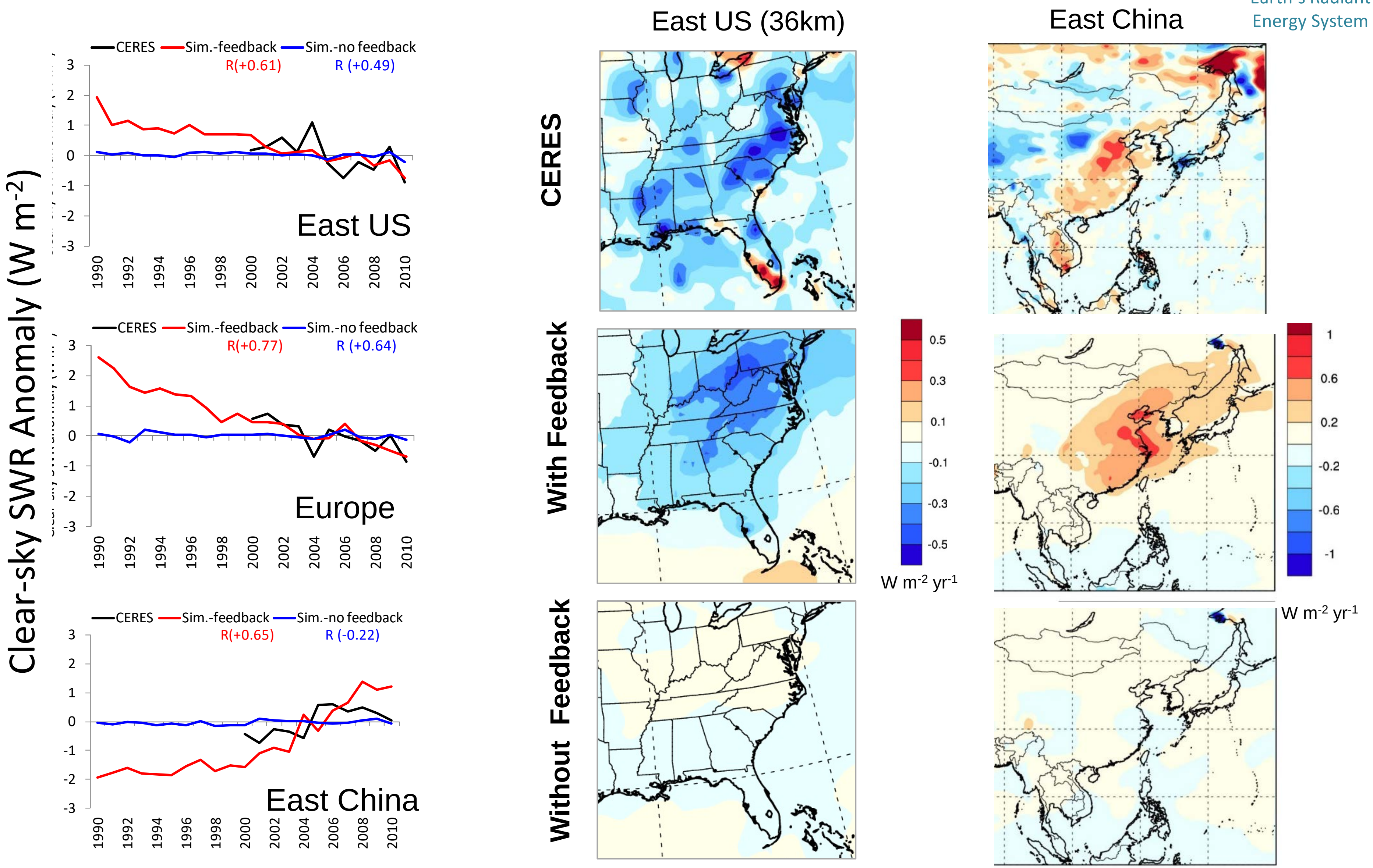


- Decreasing trends in $PM_{2.5}$, and AOD evident across the eastern U.S. in observations and model calculations
- Trends in clear-sky SW radiation show “brightening” in regions where aerosols have reduced, but are underestimated

Gan et al., 2015 (ACP)

Simulated and Observed Trends: *Clear-sky SWR at TOA (upwelling): 2000-2010*

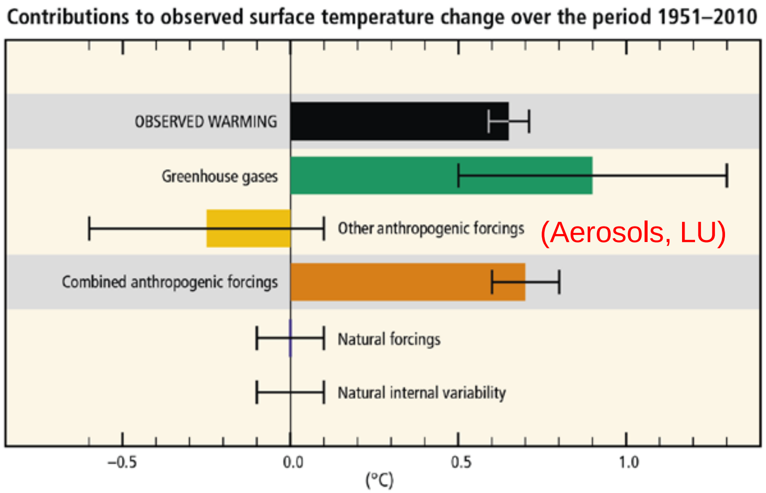
Cloud & the Earth's Radiant Energy System



- ➢ Better agreement between modeled and observed trends when aerosol feedback effects are considered
- ➢ Lack of any trend and lower R in the "no-feedback" simulation, suggest trends in clear-sky radiation are influenced by trends in aerosol burden

Impacts of Aerosol Radiative Effects on Atmospheric Dynamics, Air Pollution Exposure and Health

IPCC AR5 (2014)



Surface-cooling partially offsets GHG-related T increase

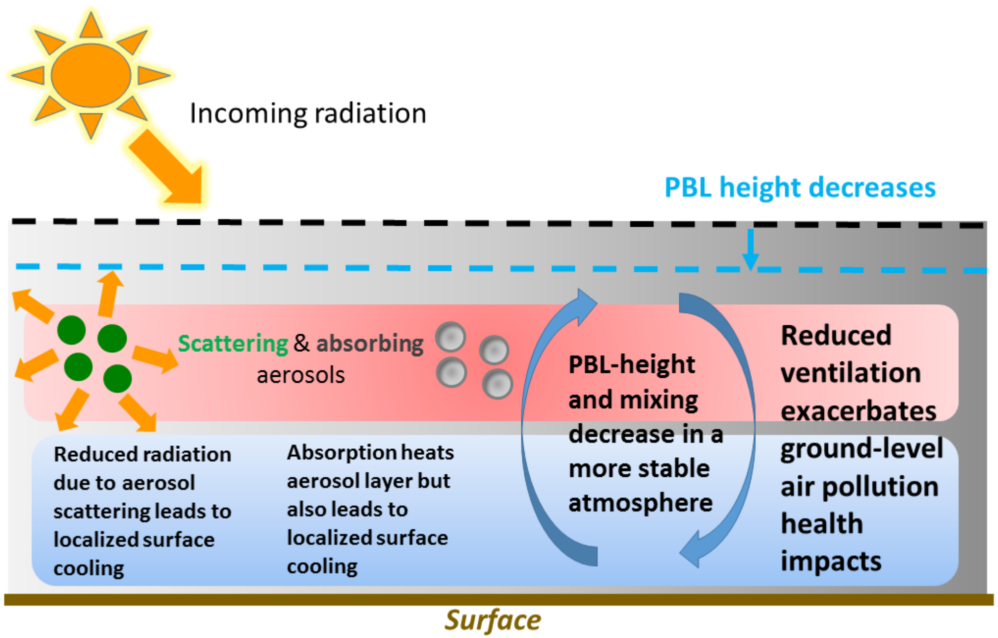
— *Is mitigating PM pollution a climate disbenefit?*

— *A cooler climate a health benefit?*

Reduced ventilation leads to a more stable atmosphere

— *Exacerbates air pollution*

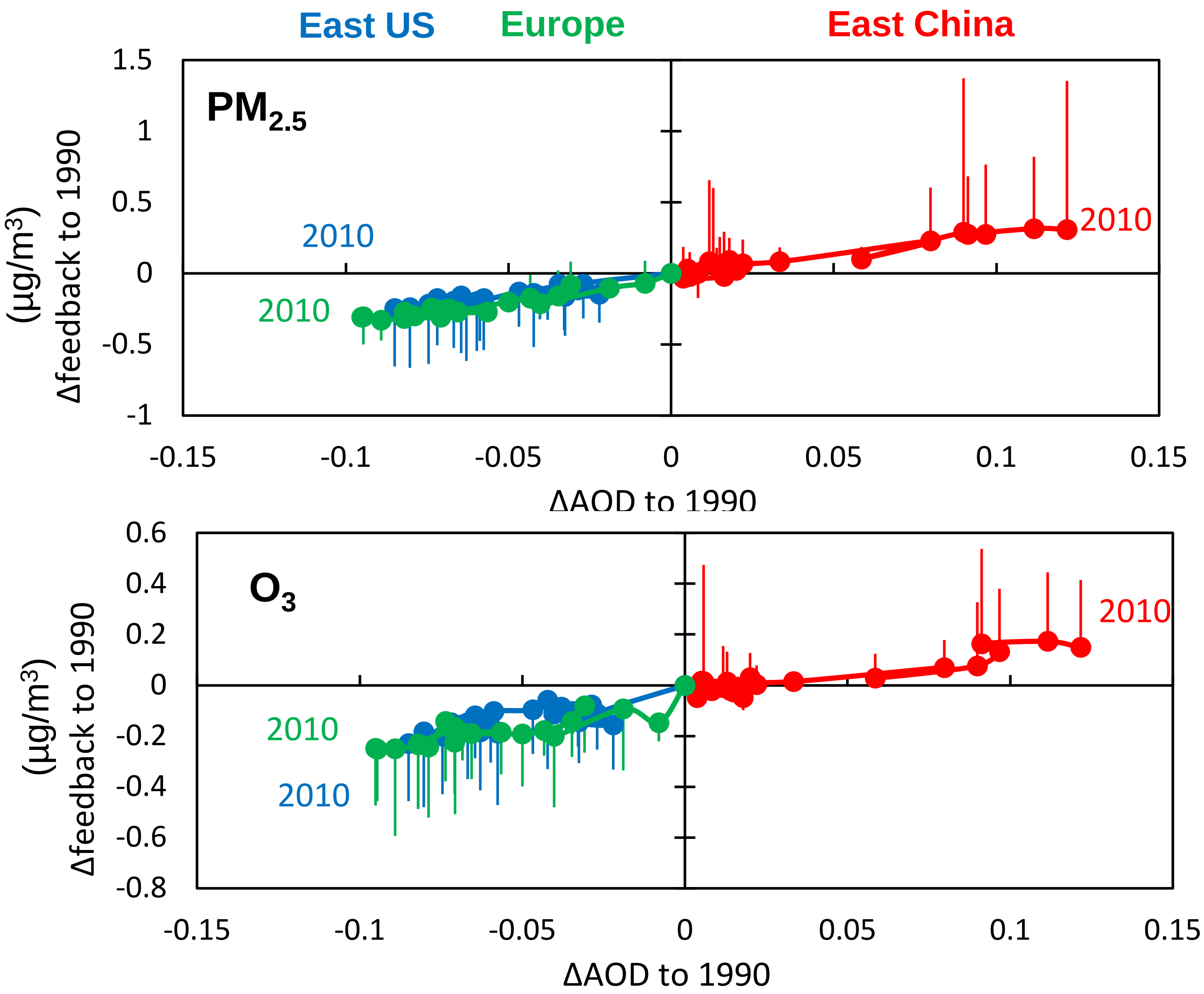
— *A health disbenefit?*



Xing et al., 2016 (ES&T)

Impact of DRE on Air Quality

Seasonal mean (dots); Maximum daily mean (bars)

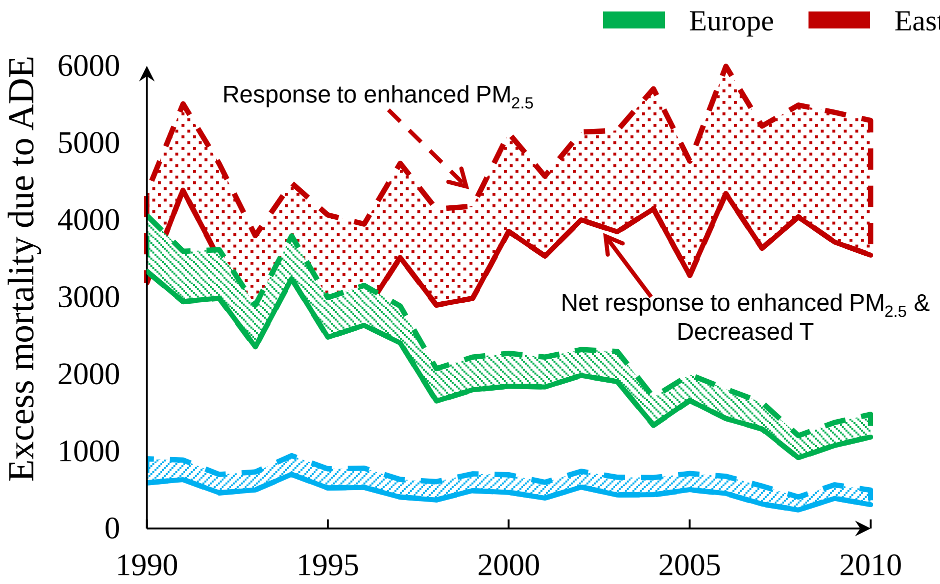


DRE impacts on cooling and ventilation impact AQ:

- *Emission Control Dividend*
- *Emissions Growth Penalty*

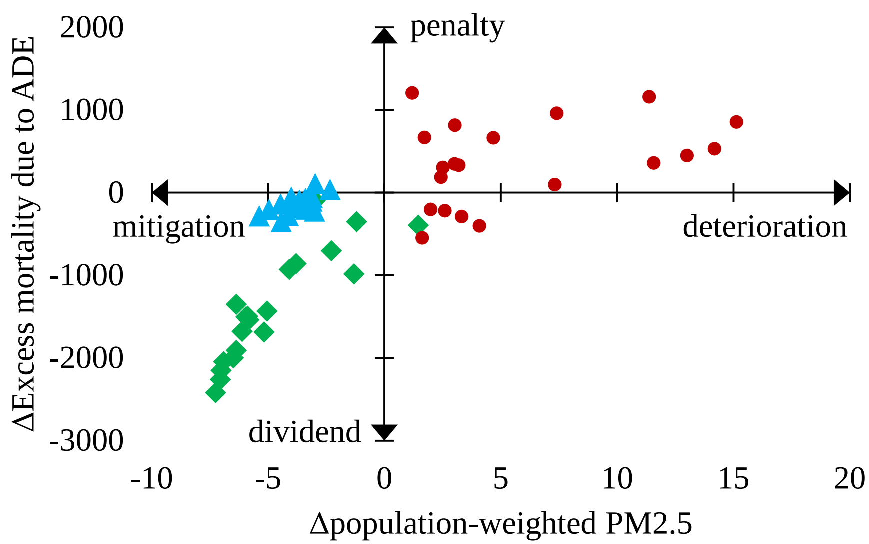
Xing et al., 2015 (JGR)

Modulation of Air Pollution Related Health Risks from Aerosol Cooling: Historical Trends in Estimated Premature Mortality



- *Health impacts from enhancement in $PM_{2.5}$ are 3-6 times larger than those reduced due to cooling*
- *ADRE related health effects have reduced by ~45-65% due to control measures in N. America and Europe*
- *Aerosol pollution control have **direct benefits** on health and **indirect benefits** on health through changes in local climate*

- *Control measures in N. America & Europe have reduced excess mortality due to ADRE – "Dividend"*
- *"Penalty" in regions witnessing increasing air pollution*

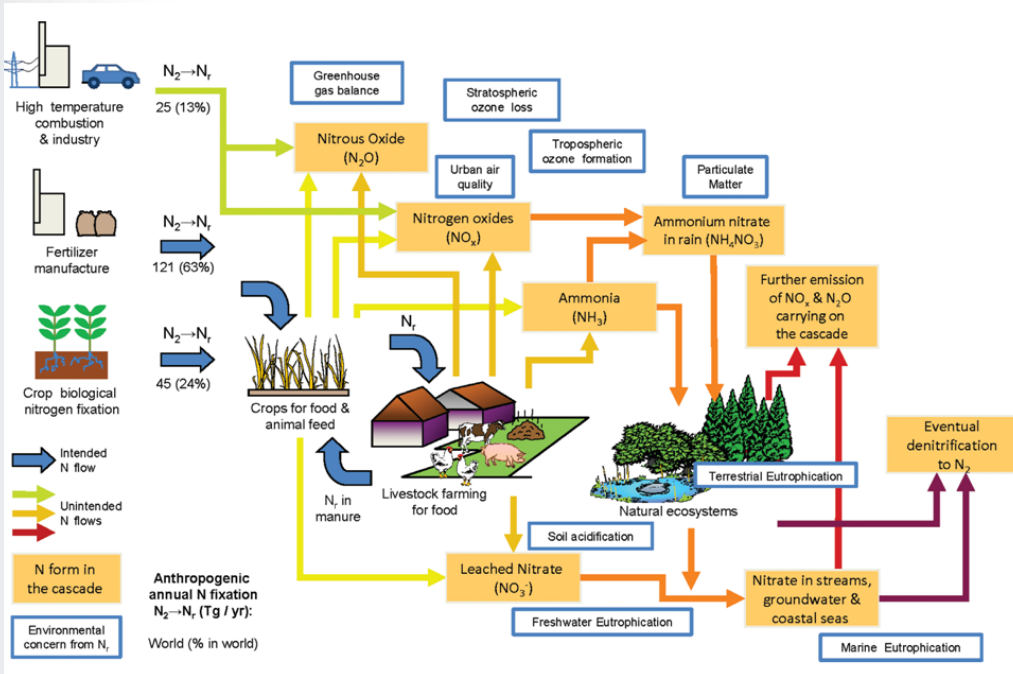


Xing et al., 2016 (ES&T)

Integrated Environmental Exposure Assessment:

Example: *Multi-Media Scenarios of Nitrogen Management in the Face of Changes in Climate & Land Use*

Integration through the Nitrogen Cascade



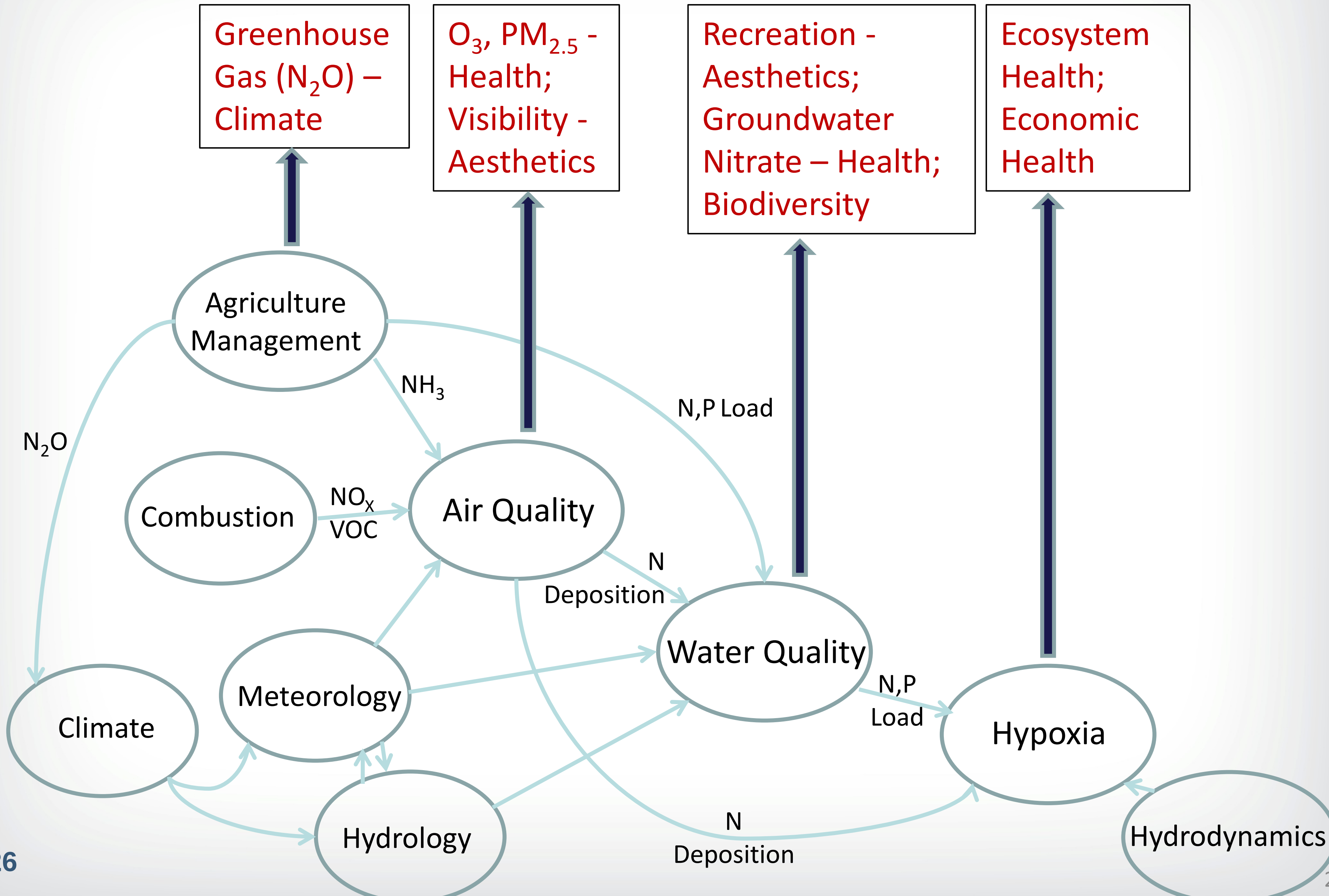
Adapted from: Galloway et al.(2003); Sutton et al. (2011):

- Nitrogen is a priority problem for Water
  - Leading cause of freshwater impairment (e.g., toxic algal blooms)
  - Major contributor to acidification of fresh waters
  - Main cause of coastal (estuarine) impairment
  - A cause of drinking water contamination
- Nitrogen air emissions impact human health (O_3 & $PM_{2.5}$) and aquatic and terrestrial ecosystems (O_3, deposition)
- *Nitrogen flow in the environment is multi-media* in character
  - Media connected by the nitrogen cascade

Regional stressors such as climate and land use changes can result in too little or too much nitrogen in the biosphere, prompting unsustainable levels of economic growth and societal behaviors that can degrade air, land and water quality.

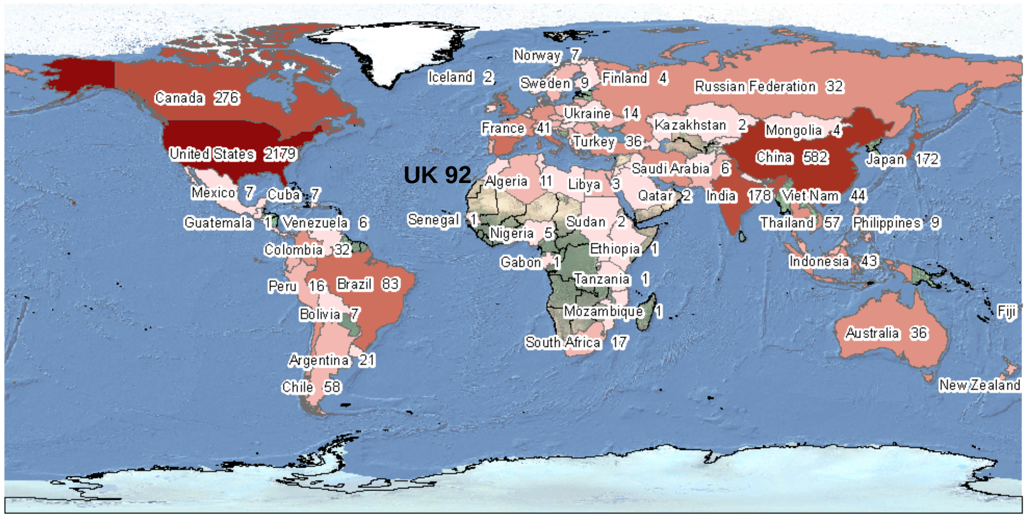
➡ Need for an integrated modeling approach: The “one-biosphere” model

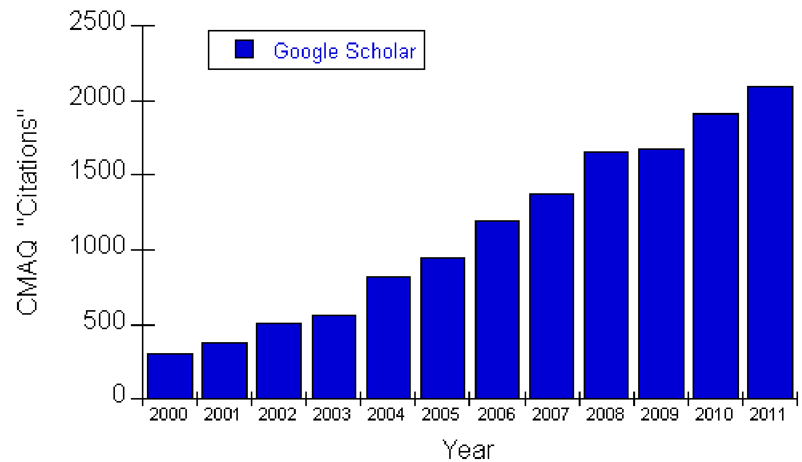
Especially for Nitrogen: Air, Land and Water are Interconnected
A One-Environment Capability Can Illuminate Win-Win Cases



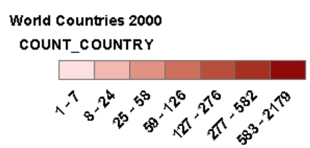
EPA United States Environmental Protection Agency

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**

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**

– **Many emerging & scientifically challenging environmental problems are at the intersection of traditional disciplinary boundaries**
  - Multiple ***inter-dependent impacts*** from stressors and potential ***unintended consequences*** of actions often arise from complex interactions and feedbacks in these systems
  - Requiring ***integration and connection of modeling systems***

❑ **Acknowledgements**

– Numerous scientists in the Computational Exposure 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/

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Extra Slides

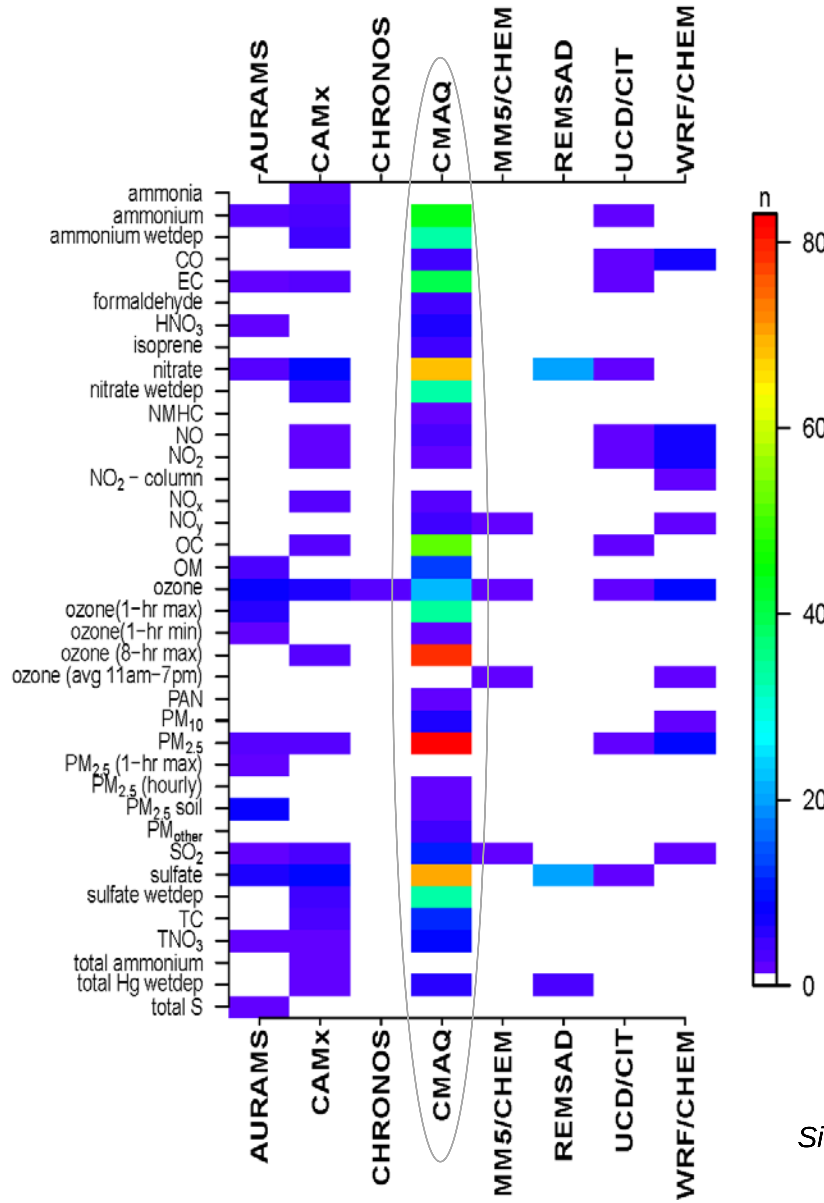
Model Evaluation Framework

- **Operational Evaluation:** *Are we getting the right answers?*
- **Dynamic Evaluation:** *Are we capturing the observed changes in air quality?*
- **Diagnostic Evaluation:** *Are we getting the right answers for the right (or wrong) reasons?*
- **Probabilistic Evaluation:** *What confidence do we have in the model predictions?*

→ Can we identify needed improvements for modeled processes or inputs?

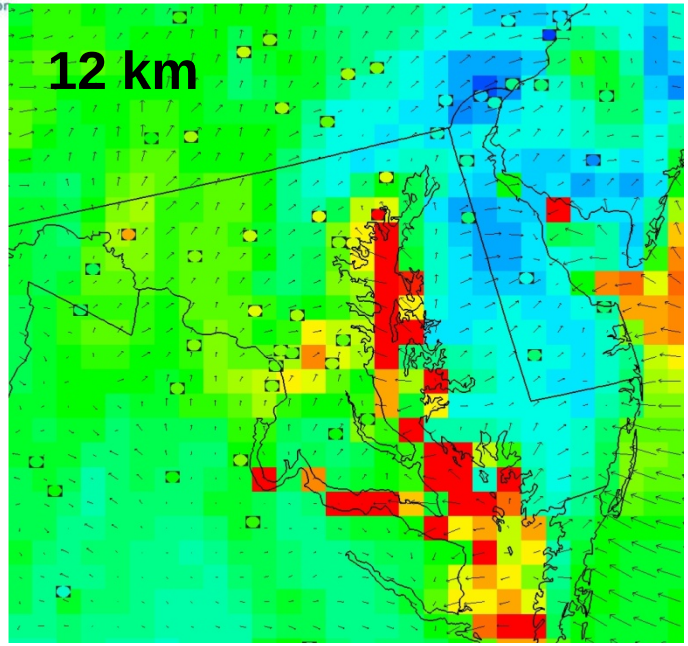
Dennis, R., T. Fox, M. Fuentes, A. Gilliland, S. Hanna, C. Hogrefe, J. Irwin, S.T. Rao, R. Scheffe, K. Schere, D. Steyn, and A. Venkatram: A framework for evaluating regional-scale numerical photochemical modeling systems, Environ. Fluid Mech., DOI 10.1007/s10652-009-9163-2, 2010.

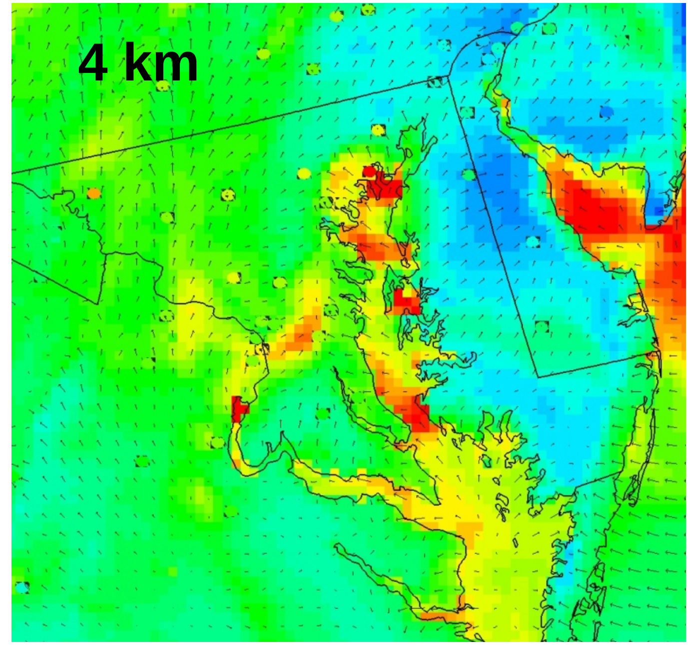
CMAQ
Growing number of model evaluation studies



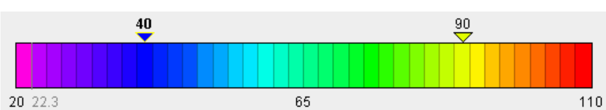
Simon et al., Atmos. Env. 2012

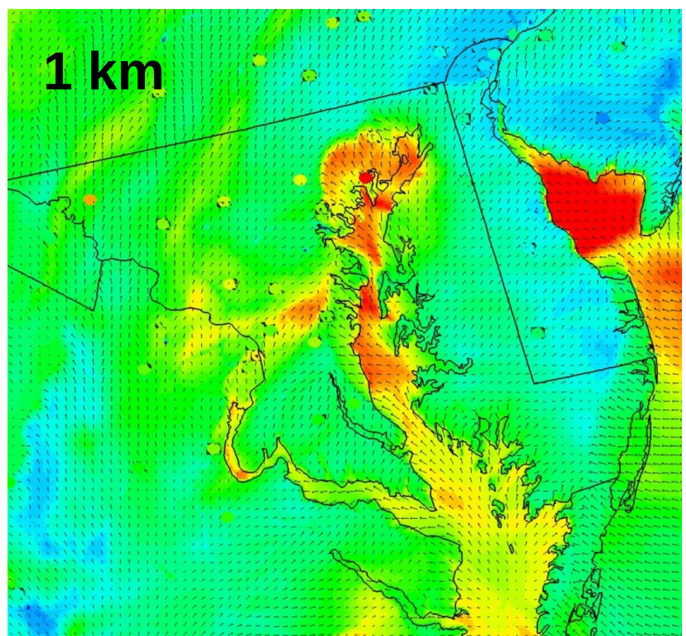
Emerging need: Improvements in Fine-scale simulations





O_3 at 3pm LT



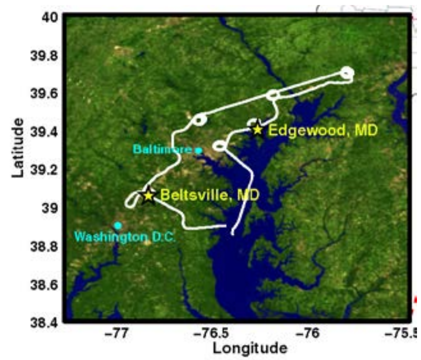


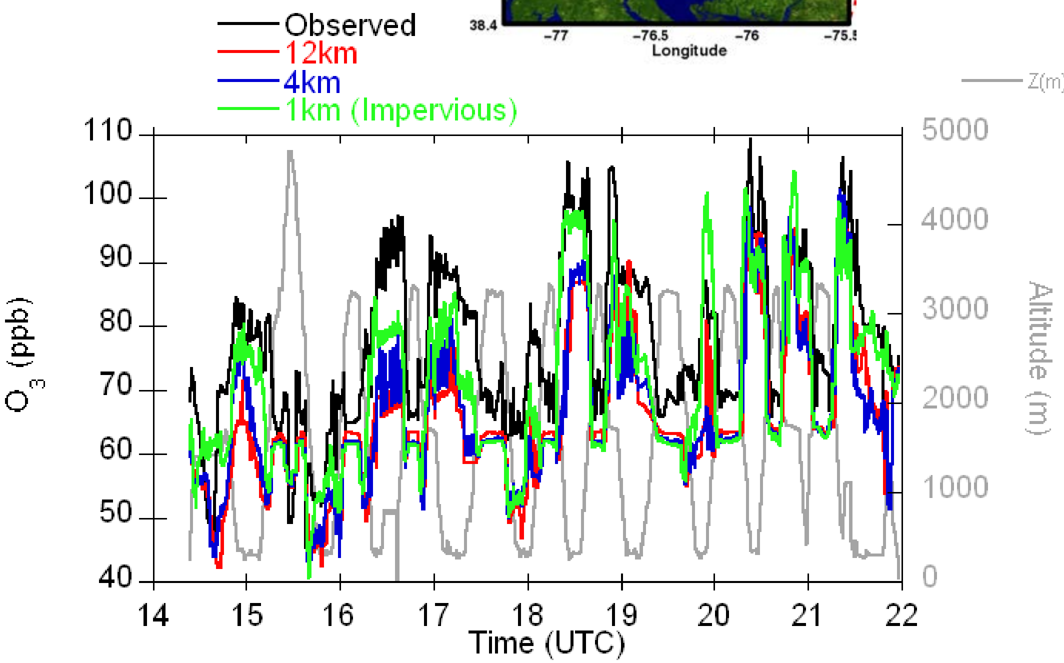
Representing spatial gradients

- Bay breeze impacts on inland monitors

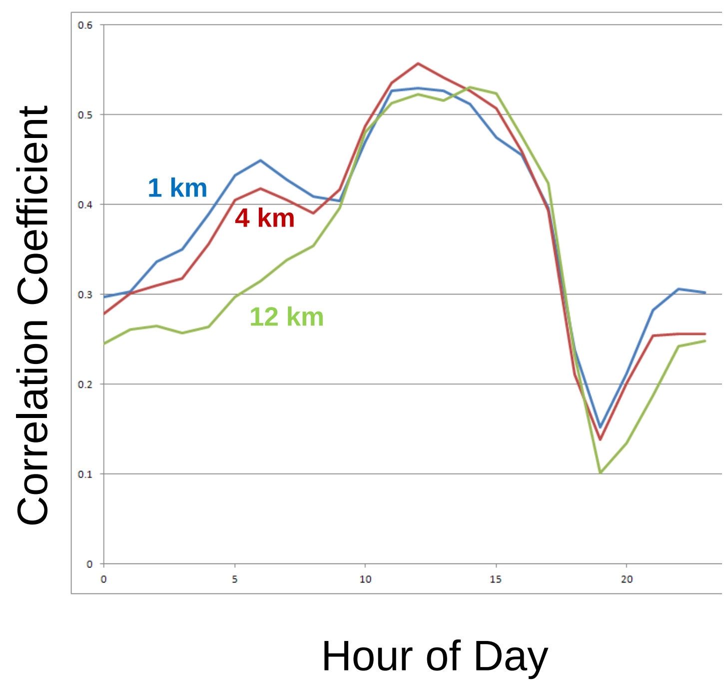
Improvements in Fine scale simulations

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



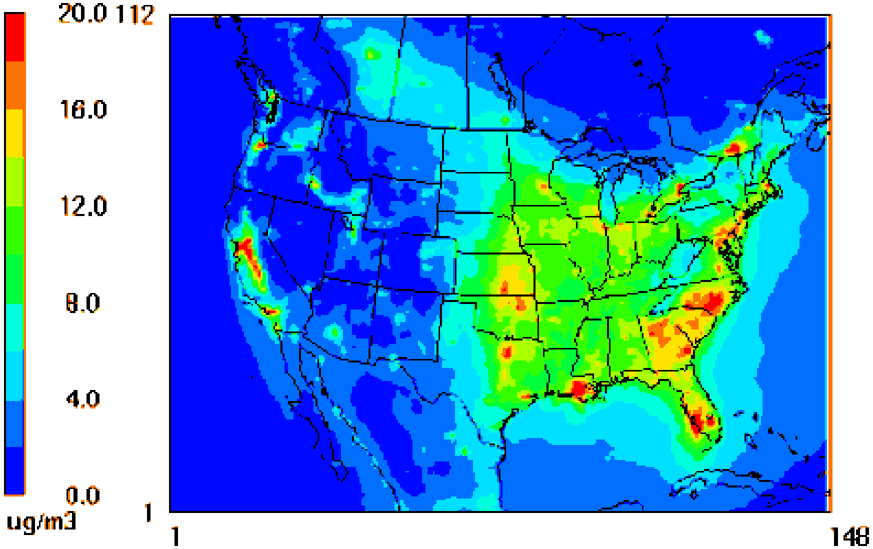
Sensitivity Analysis: Direct Decoupled Method

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.)

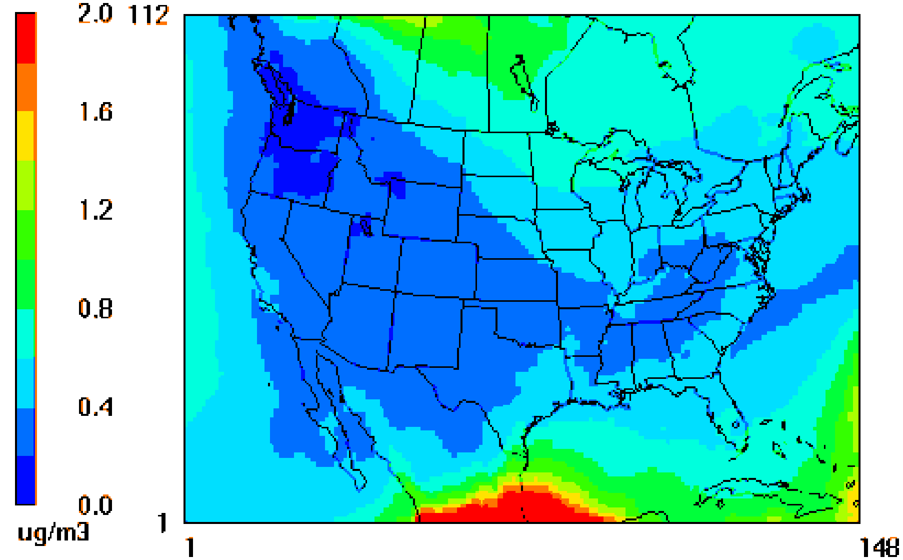
Sensitivity of species *i* to model parameter *j*:

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

January $PM_{2.5}$



$PM_{2.5}$: LBC Contribution

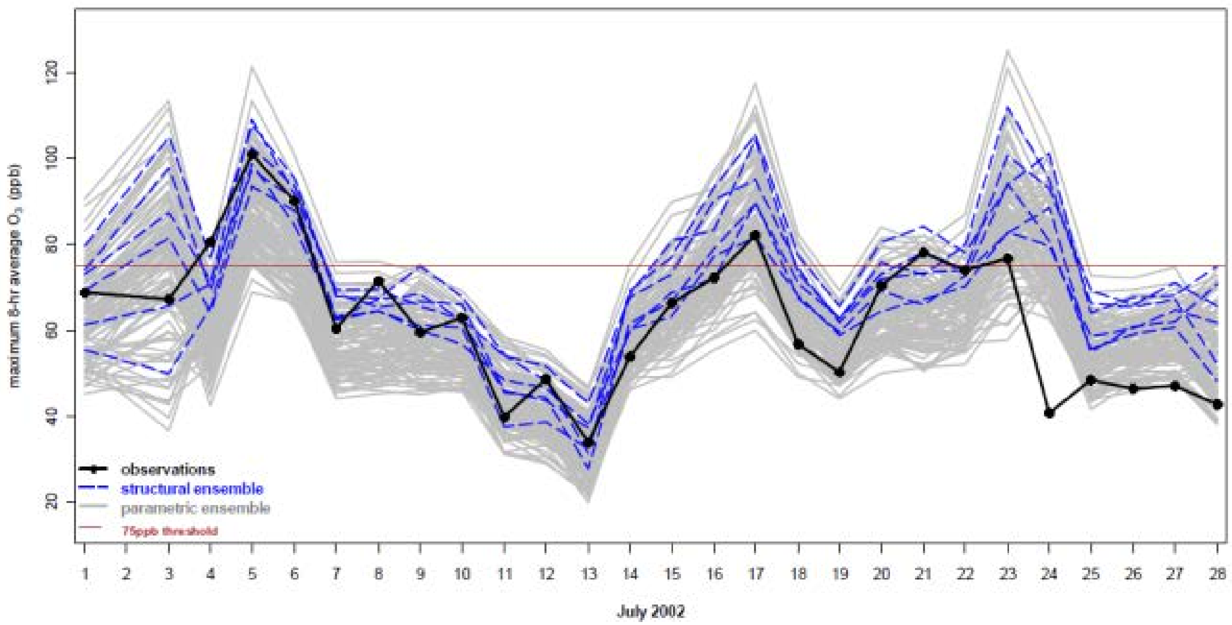


Courtesy: Sergey Napelenok

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.

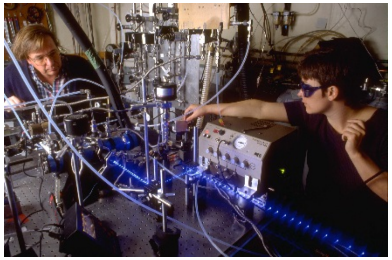
Courtesy: Kristen Foley

Background

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

- ***Scientific efforts to understand these have involved a combination of:***

  - **Laboratory Experiments**
    - Provide basic data on 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 conditions at particular time & location

  - **Modeling Experiments**
    - Tools to integrate and synthesize our evolving knowledge of various atmospheric processes