Applying Data Assimilation and Adjoint Sensitivity to Epidemiological and Policy Studies of Airborne Particulate Matter

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Contributors

- Faculty at Iowa
  - Gregory Carmichael
  - Naresh Kumar
  - R. William Field
  - Jacob Oleson
- Postdoctoral Researchers
  - Scott Spak
  - Sang Rin Lee
- Faculty at University of Ottawa
  - Daniel Krewski
- Graduate Students
  - Sinan Sousan
- Undergraduate Students
  - Adam Beranek-Collins

- Iowa / Ottawa project is a model development and proof of concept work focused on:
  - Data fusion (AQS / MODIS / CMAQ)
    - For total and source-tagged PM2.5
  - Demonstration of data fusion outdoor PM estimates in health studies
  - Demonstration of target-oriented sensitivity approach

Intellectual Acknowledgements

- Seeds of these ideas planted by many
  - Greg Carmichael (Co-I), Bill Field (Co-I), Dan Krewski (Co-I)
  - Ted Russell (AAAR Plenary on model data fusion, 2006)
  - Tiafeng Chai
  - Pioneers and authors of key data assimilation advances
    - Adrian Sandu, Amir Hakami, Daven Henze, John Seinfeld, Bhupesh Adhikary, Youhua Tang

Why are data fusion approaches to the aerosol-health problem required?

Fine-Particulate Air Pollution and Life Expectancy in the United States

C. Arden Pope III, Ph.D., Majid Ezzati, Ph.D., and Douglas W. Dockery, Sc.D.

NEJM 2009; 360: 376-86.

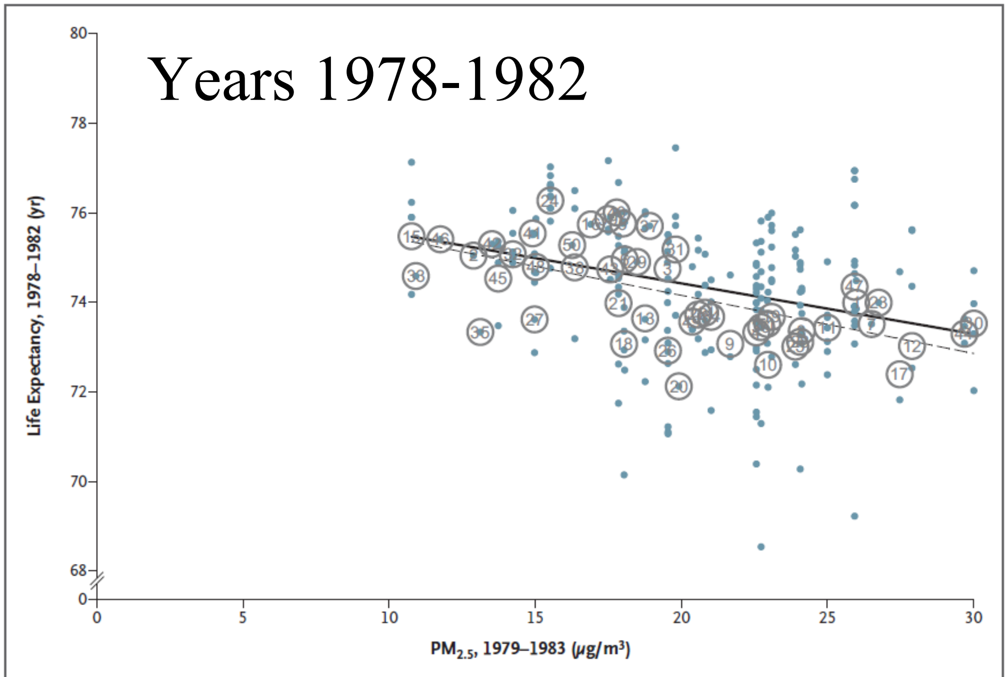

Figure 2. Cross-Sectional Life Expectancies for 1978–1982, Plotted against $PM_{2.5}$ Concentrations for 1979–1983.

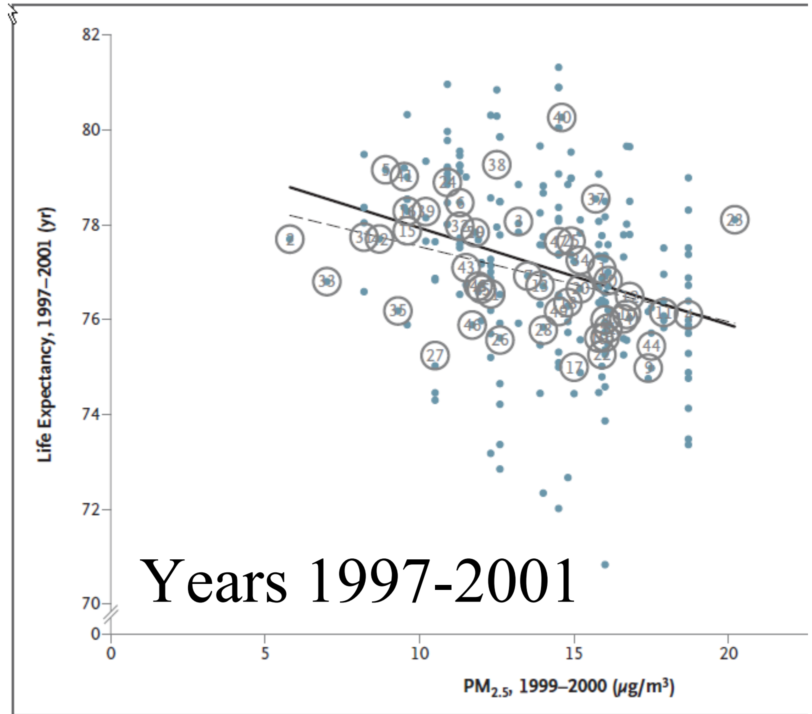

Figure 3. Cross-Sectional Life Expectancies for 1997–2001, Plotted against $PM_{2.5}$ Concen

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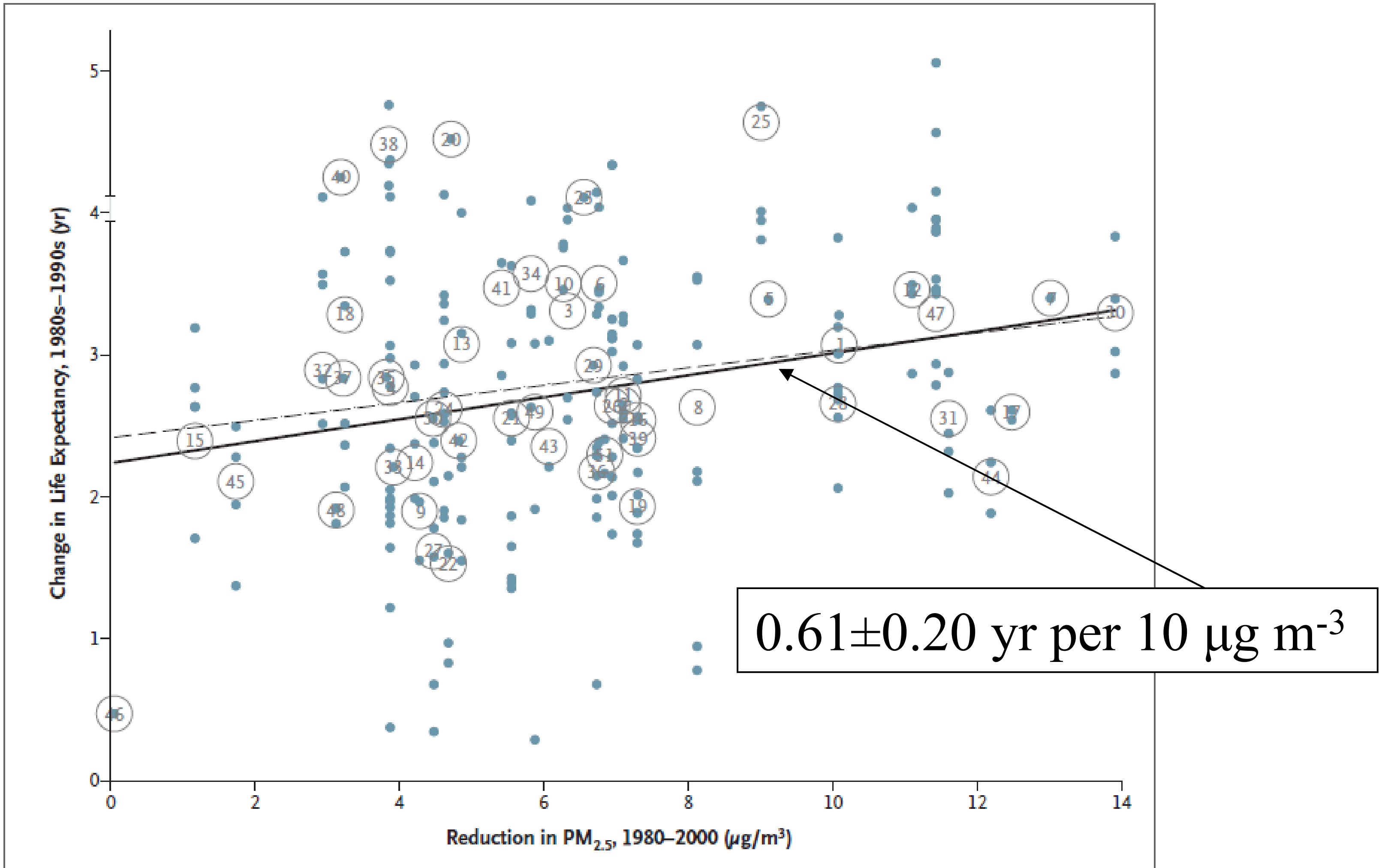

Figure 4. Changes in Life Expectancy for the 1980s–1990s, Plotted against Reductions in $PM_{2.5}$ Concentrations for 1980–2000.

Approximate cost benefit of further reductions in premature death vs. PM control

- Use 0.61year per 10 μg m^{-3} (Pope et al. NEJM)
- Scenario I – NOx and SO_2 controls
  - Pinder et al. (2007)
    - 20% reduction in $PM_{2.5}$ in Eastern U.S. through lowest cost NO_x / SO_2 program is ~$9B per year and achieves ~3 μg m^{-3} reduction
- Net result
  - extend average lifespan by 0.2 years at a cost of ~$2000 per person
    - ~$30 per day of increased lifespan

Pinder & Adams (2007) ES&T (41)

- Repeat for Clean Diesel Rule using EPA Impact Assessment

	SOx/NOx	DPM
Reduction	~3 μg m^{-3}	0.27-0.65 μg m^{-3}
Added lifetime	0.2 yr	0.04 yr
Cost per person	$2000	$1000

EPA Regulatory Impact Assessment, 2000
EPA420-R-00-026, December 2000

- Important features
  - Exposure misclassification
    - e.g.
      - Intake fraction of large electric power stations ~ 0.8 per million (kg inhaled vs. kg emitted)
      - Intake fraction of vehicles 7-21 per million
  - Particle Component Toxicity Problem
  - Variability in Population Sensitivity

Marshall et al. (2005) Atmos. Environ.; Heath et al. (2006) Atmos. Environ.

Component Toxicity Problem

- A growing body of acute animal studies, human studies, Concentrated Atmospheric Particle (CAPs) studies, and tissue culture studies

Circulating Biomarkers of Inflammation, Antioxidant Activity, and Platelet Activation Are Associated with Primary Combustion Aerosols in Subjects with Coronary Artery Disease

Ralph J. Delfino,[1] Norbert Staimer,[1] Thomas Tjoa,[1] Andrea Polidori,[2] Mohammad Arhami,[2] Daniel L. Gillen,[3] Micheal T. Kleinman,[4] Nosratola D. Vaziri,[5] John Longhurst,[5] Frank Zaldivar,[6] and Constantinos Sioutas[2]

  - Elderly panel of 29 subjects with coronary artery disease; blood and air quality monitored for 12 weeks

Environ. Health Perspect. (2008) 116(7)

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		$PM_{0.25}$	$PM_{0.25\text{-}2.5}$	PM_{coarse}	EC	$EC_{o\text{-}o}$	OC	OC_{pri} $OC_{pri\text{-}o\text{-}o}$	PN	$PN_{o\text{-}o}$	CO	NO2	SOA
Associated with heart attack risk	Outdoor vs. CRP	Yellow	Grey	Blue	Yellow	White	Grey	Yellow	Yellow	White	Yellow	Yellow	Grey
	Outdoor vs. IL-6	Yellow	Grey	Grey	Yellow	White	Grey	Yellow	Yellow	White	Yellow	Yellow	Grey
	Outdoor vs. sTNF-RII	Yellow	Grey	Blue	Yellow	White	Blue	Yellow	Yellow	White	Yellow	Yellow	Grey
	Indoor vs. CRP	Blue	Blue	Blue	Blue	Yellow	Grey	Yellow	Yellow	Yellow	Yellow	Yellow	Grey
	Indoor vs. IL-6	Grey	Grey	Grey	Yellow	Yellow	Grey	Yellow	Yellow	Yellow	Yellow	Yellow	Grey
	Indoor vs. sTNF-RII	Grey	Grey	Grey	Yellow	Yellow	Grey	Yellow	Yellow	Yellow	Yellow	Grey	Grey
Oxidative Stress	Outdoor sP-selectin	Grey	Yellow	Grey	Yellow	White	Grey	Yellow	Grey	White	Grey	Grey	Grey
	Indoor sP-selectin	Blue	Grey	Yellow	Yellow	Yellow	Blue	Yellow	Grey	Blue	Blue	Yellow	Grey
	Outdoor Cu,Zn-SOD	Yellow	Blue	Blue	Yellow	White	Blue	Yellow	Blue	White	Yellow	Yellow	Grey
	Indoor Cu,Zn-SOD	Blue	Blue	Blue	Yellow	Yellow	Blue	Yellow	Grey	Blue	Yellow	Yellow	Grey

Yellow = highest correlation. Blue = lower correlation. Grey = zero or negative correllation. Other biomarkers with positive but statistically nonsignificant biomarkers.

	$PM_{0.25}$	$PM_{0.25-2.5}$	PM_{coarse}	EC	EC_{o-o}	OC	OC_{pri} $OC_{pri-o-o}$	PN	PN_{o-o}	CO	NO2	SOA
Associated with heart attack risk: Outdoor vs. CRP												
Outdoor vs. IL-6												
Outdoor vs. sTNF-RII												
Indoor vs. CRP												
Indoor vs. IL-6												
Indoor vs. sTNF-RII												
Oxidative Stress: Outdoor sP-selectin												
Indoor sP-selectin												
Outdoor Cu,Zn-SOD												
Indoor Cu,Zn-SOD												

Yellow = highest correlation. Blue = lower correlation. Grey = zero or negative correllation. Other biomarkers with positive but statistically nonsignificant biomarkers.

Applying Data Assimilation and Adjoint Sensitivity to Epidemiological and Policy Studies of Airborne Particulate Matter

- **Objective 1**: Evaluate **data assimilation (DA)** methods for data fusion of CMAQ with
  - **AQS PM2.5 and speciated PM2.5**
  - **MODIS Aerosol Optical Depth / Aeronet Optical Depth**
  - **Methods to be developed for total PM2.5 and source-tagged PM2.5 model versions**

- **Objective 2**: Apply PM2.5 from objective 1 to pilot epidemiological analyses

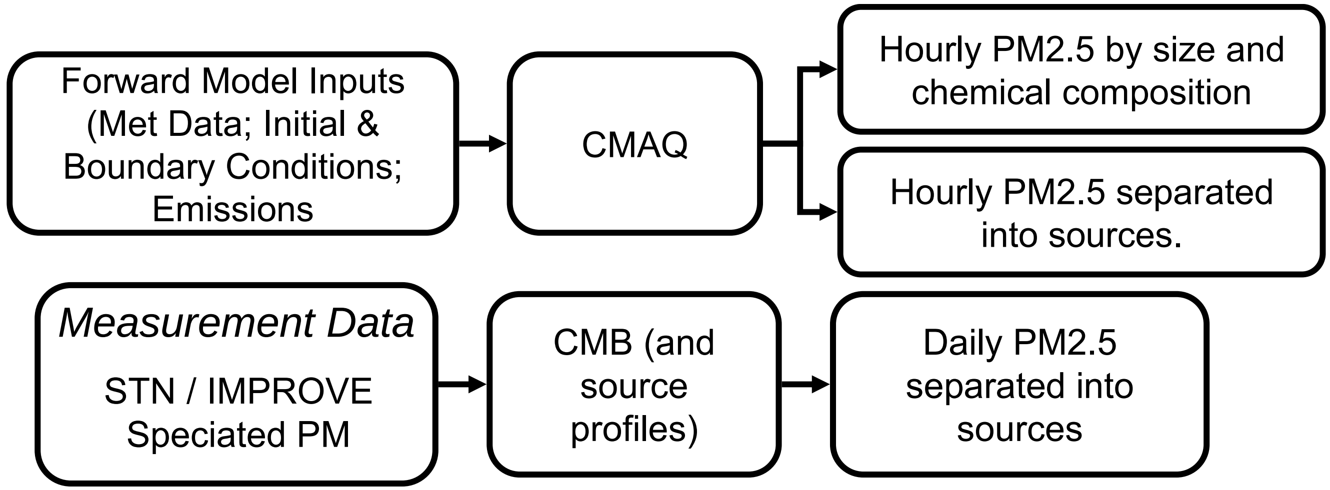
- **Objective 3** – Demonstrate the utility of target-oriented and adjoint sensitivity methods for visualization of relationships between user-defined air quality/health targets and spatially-resolved emissions.

Objective 1 – Modeling and Data Assimilation

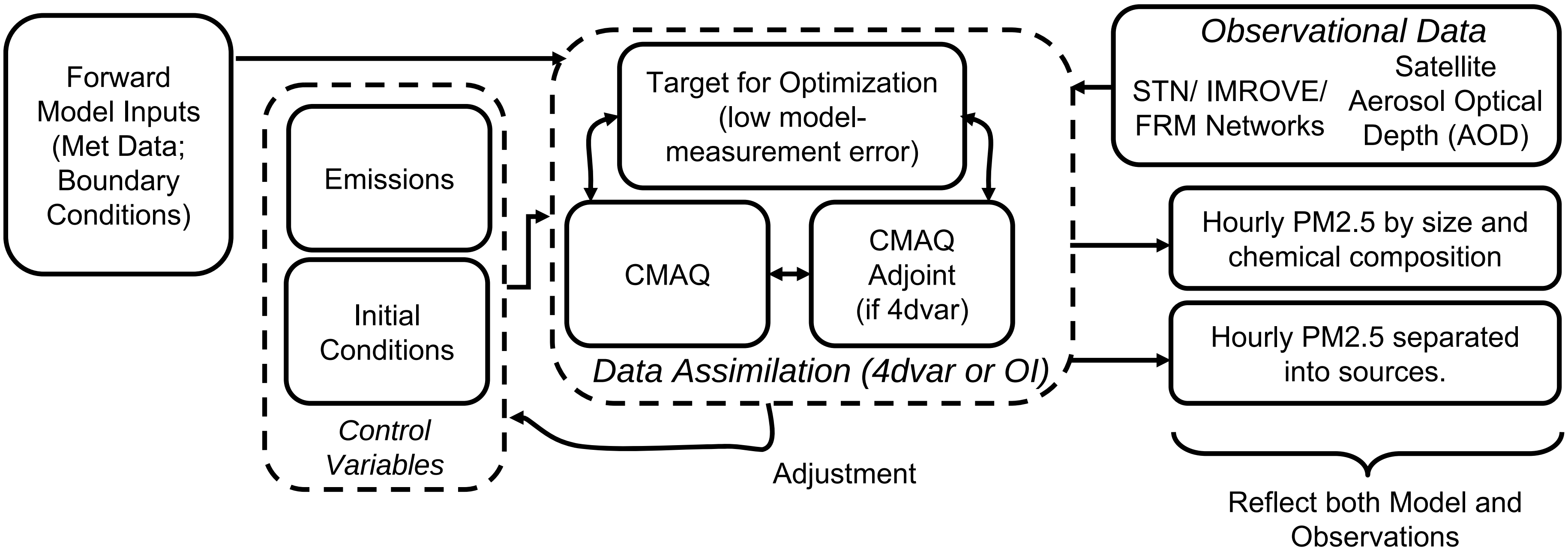
- Compare exposure estimates developed by three methods:
  - (a) model approach using source-oriented modeling with CMAQ;
  - (b) observational approach relying on CMB source-attribution of speciated filter samples; and
  - (c) hybrid analysis combining source-oriented modeling with speciated measurements through data assimilation (DA)

Source-Oriented Modeling

Source-Receptor Analysis



II – Model-Measurement Hybrid (Data Assimilation)



Summary of previous assimilation results

- Adhikary et al. (Atmos. Environ. 2008)
- A regional scale chemical transport modeling of Asian aerosols with data assimilation of AOD observations using optimal interpolation technique
- Improving analysis state (not forecast) PM2.5 estimates at two sites by assimilating satellite AOD measurements
- OI run at daily time step with OI result feeding next day's model prediction, and at monthly time step
- Up to 50% reduction in RMSE due to ability to correct uncertain dust contributions to $PM_{2.5}$

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Impact of Daily MODIS Assimilation on Predicted PM 2.5

B. Adhikary et al. / Atmospheric Environment 42 (2008) 8600–8615

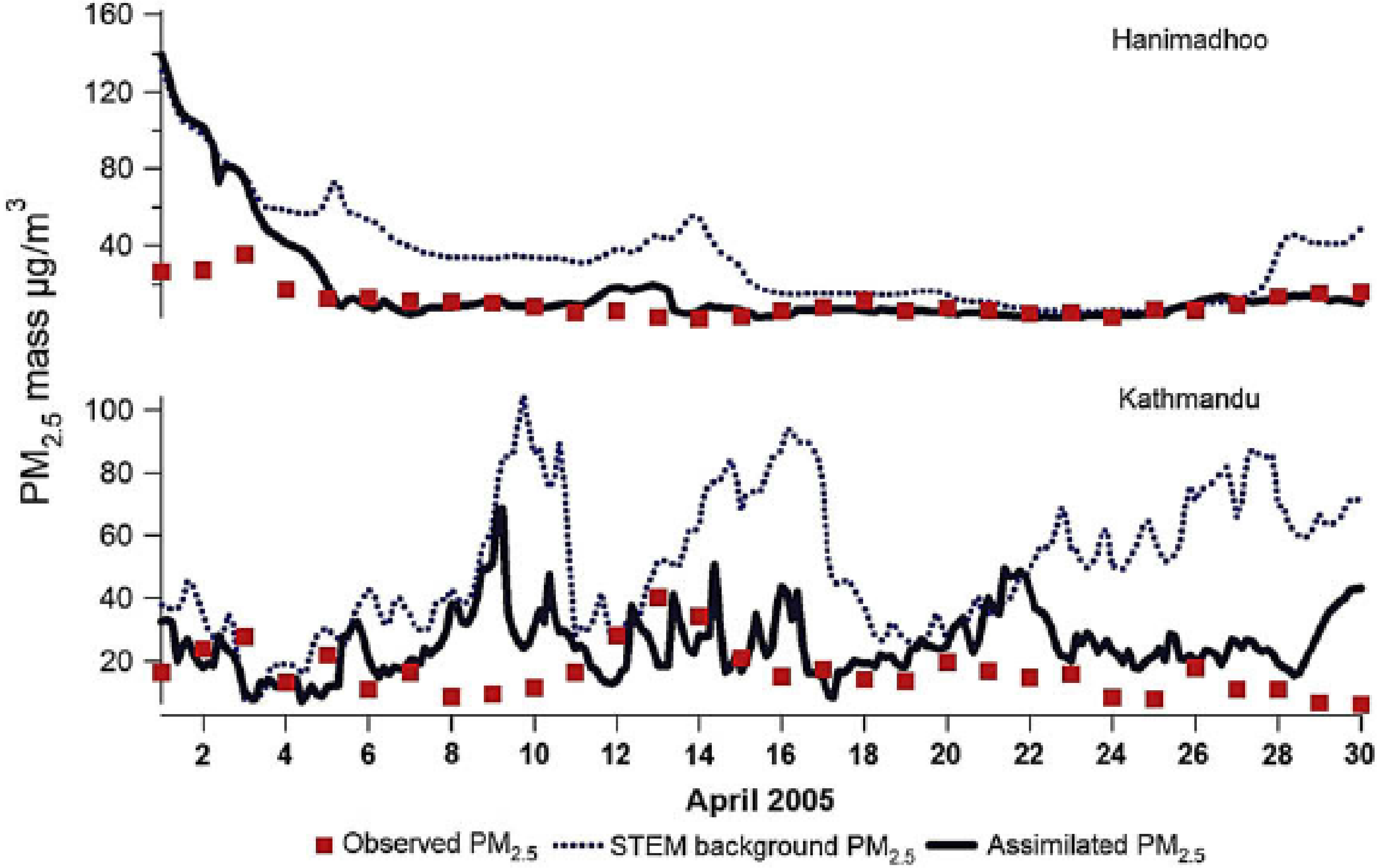

Fig. 3. Comparison of $PM_{2.5}$ mass at ABC stations.

Summary of previous assimilation results

- Tombetter et. Al. (ACP, 2009)
  - PM10 Data Assimilation over Europe with OI method
    - Focused on improving PM10 forecasts using daily OI to improve initial conditions of PM10 for next day
    - Assimilated surface measurements
    - Decrease in RMSE of 1.5 µg m^{-3} (PM2.5 and PM10 levels ~20 µg m^{-3}) and 10% increase in correlation)

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Summary of previous assimilation results

- Pan et al. (Atmos. Environ. 2007)
  - Top-down estimate of mercury emissions in China using four-dimensional variational data assimilation
  - Improving analysis state (not forecast) of aircraft Hg measurements using STEM adjoint, and control variable of gridded Hg emissions

Others assimilation examples

- Hakami et al., Adjoint inverse modeling of black carbon during the Asian Pacific Regional Aerosol Characterization Experiment. Journal Of Geophysical Research-Atmospheres, 2005. **110**(D14).
- Barbu et al., A multi-component data assimilation experiment directed to SO2 and sulfate over Europe. Atmos. Environ (2009).
- Satellite AOD data assimilation methods exploited in recent U Iowa work
  - Yu et al., Annual cycle of global distributions of AOD from integration of MODIS retrievals and GOCART model simulations. JGR (2003).
  - Nui et al., DA of dust aerosol observations for CUACE/dust forecasting system. ACPD (2007).
  - Collins et al. Simulating aerosols using a chemical transport model with assimilation of satellite aerosol retrievals: methodology for INDOEX. JGR (2001).
  - Wang et al. GOES 8 aerosol optical thickness assimilation in a mesoscale model. JGR (2004).

MODIS AOD & CMAQ

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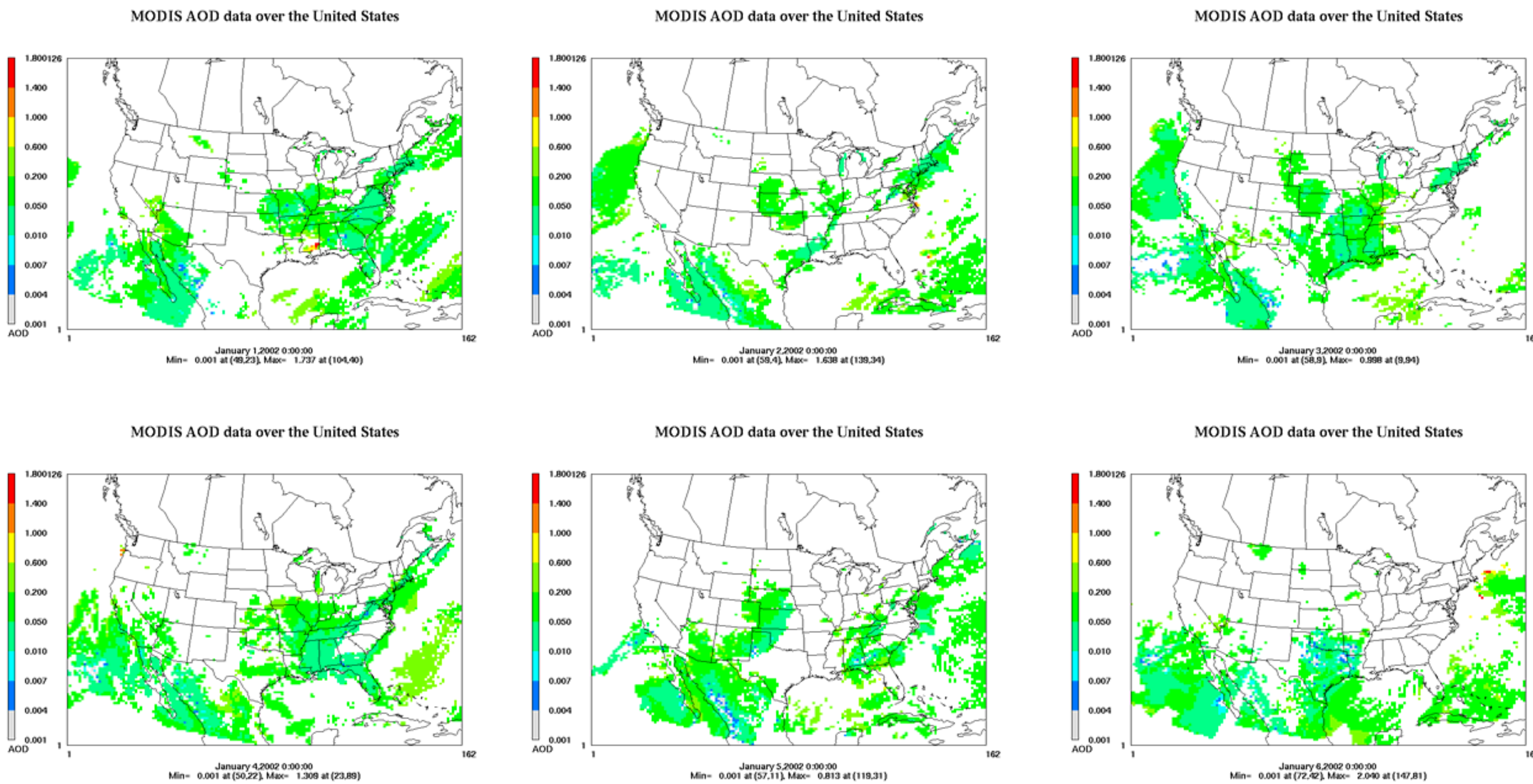
Daily MODIS AOD



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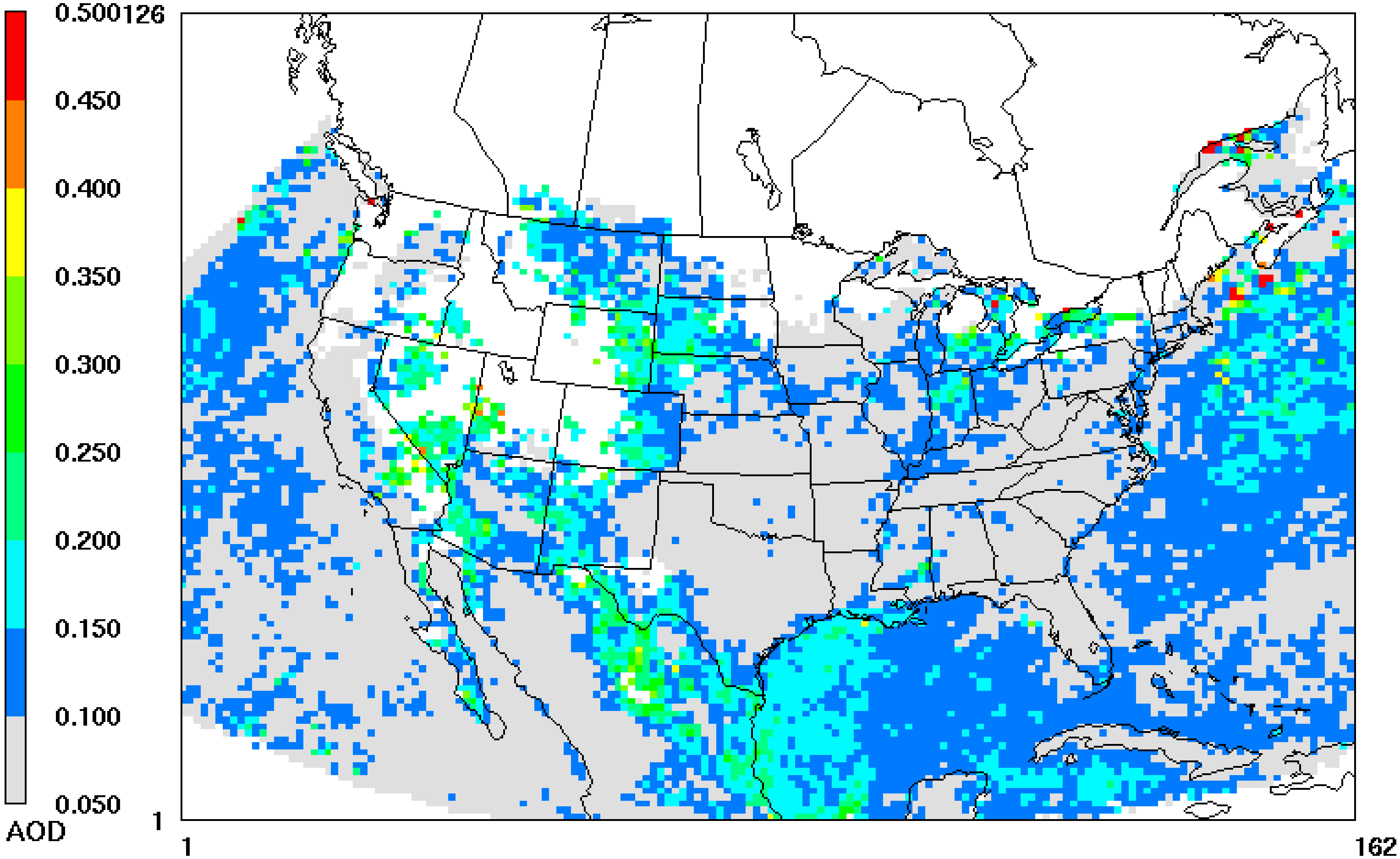
January 2002 – MODIS AOD Average



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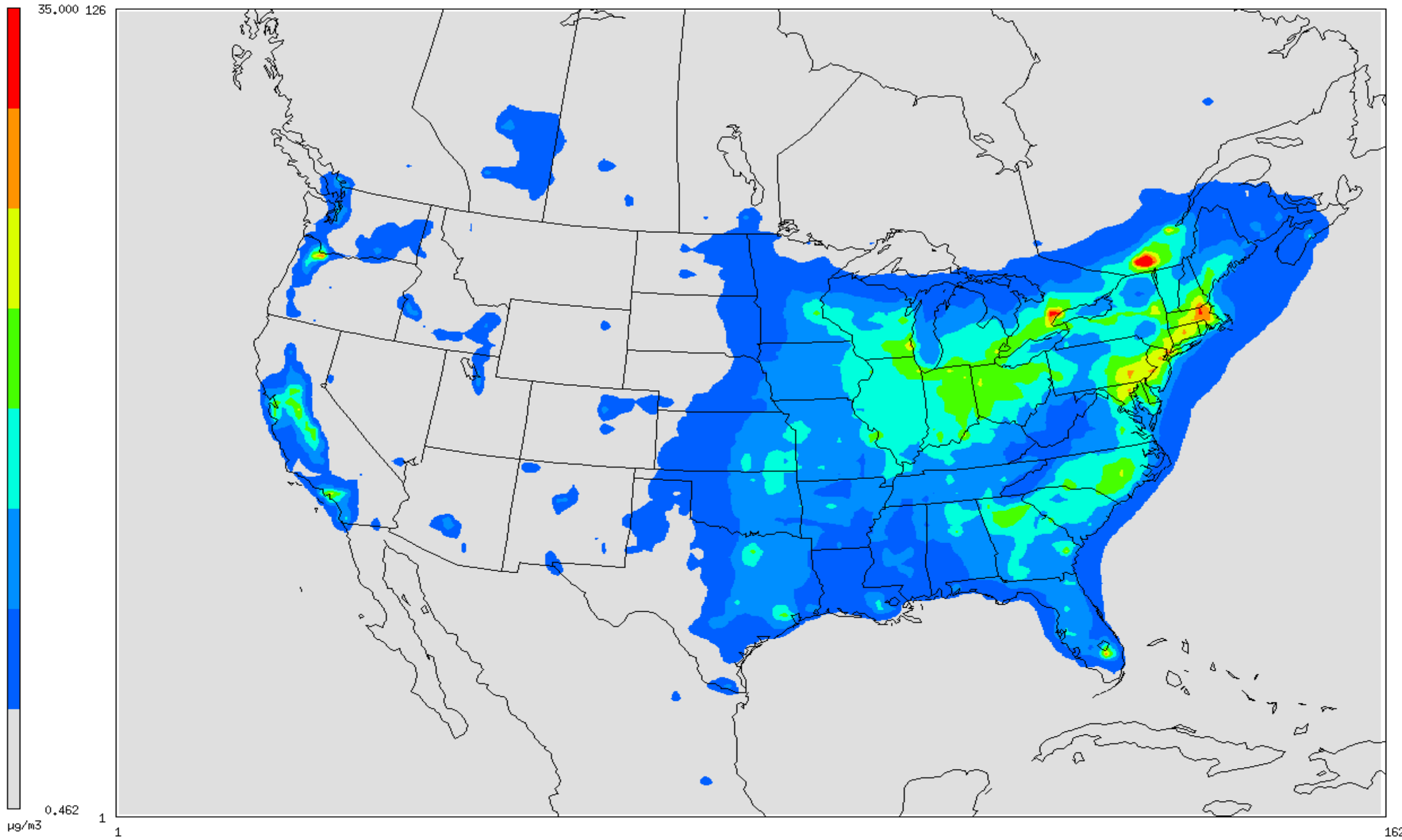
Jan 2002 CMAQ Surface PM2.5 Map



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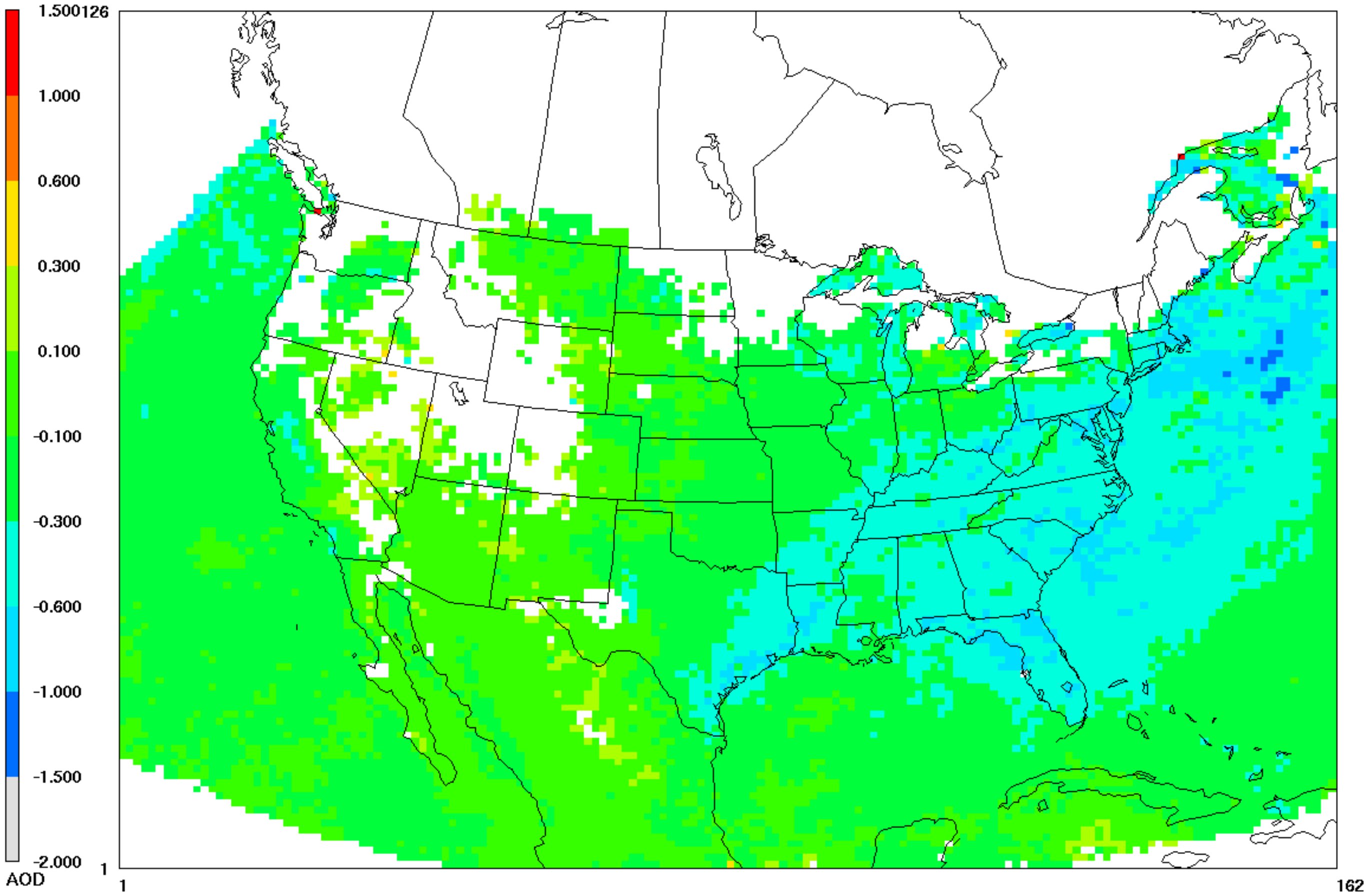
January 2002: CMAQ - MODIS AOD
All pairwise differences averaged



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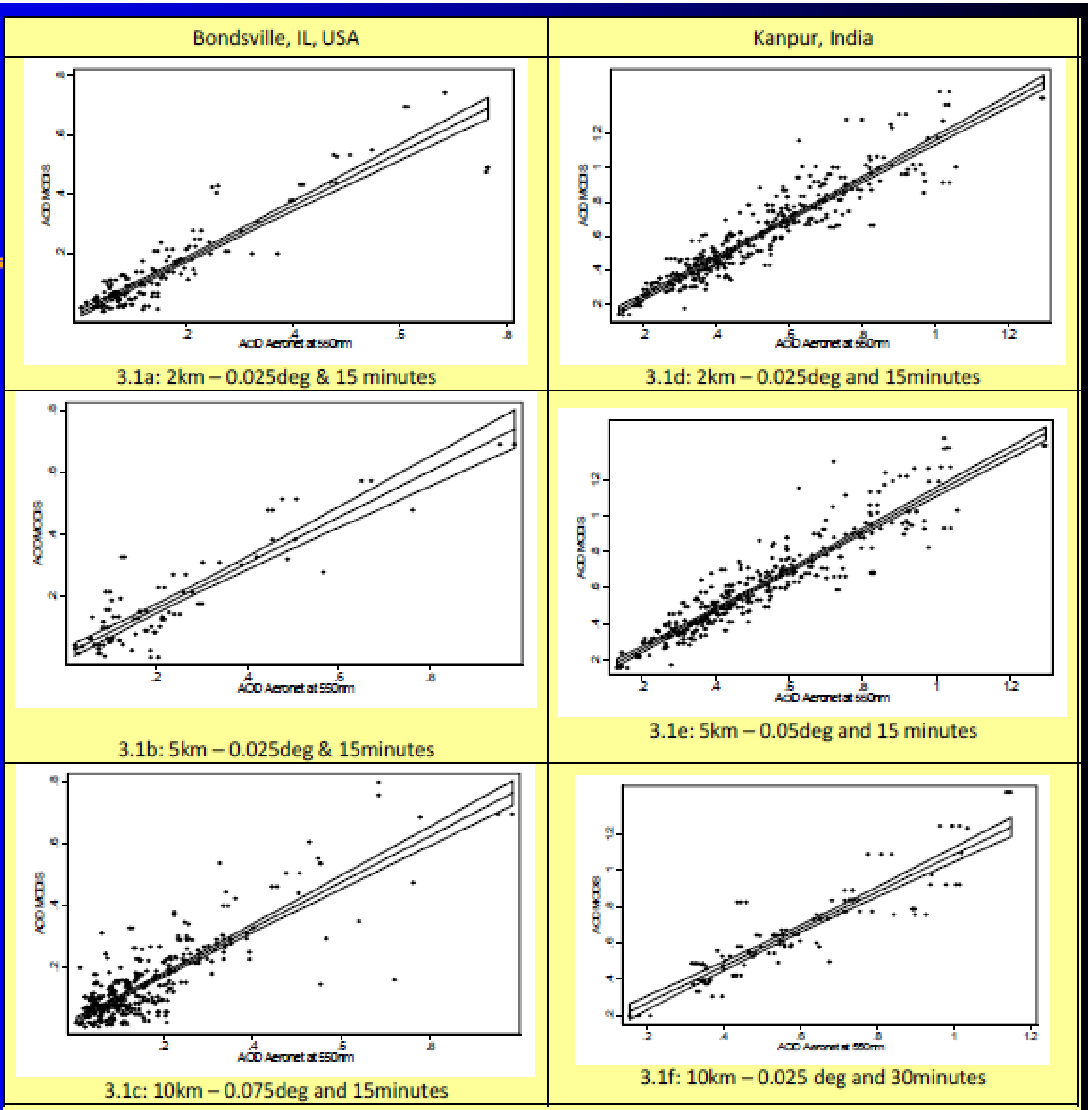
- Next steps for total $PM_{2.5}$
  - apply the OI algorithm $\tau_m^{'} = \tau_m + K(\tau_o - H\tau_m)$
  - apply the speciation adjustments developed at Iowa (fine mode AOD impacts sulfate and OC, while total AOD – fine mode AOD impacts dust)
  - add surface PM2.5 to optimal interpolation

Multi-resolution AOD retrieval



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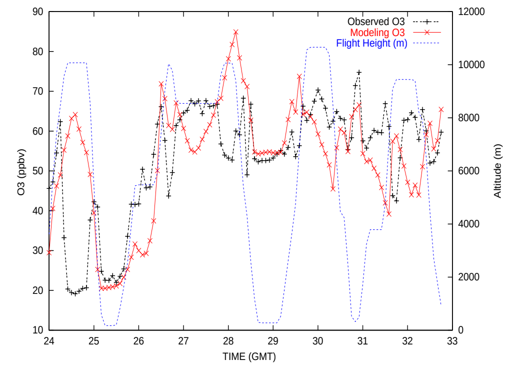
Advanced Data Assimilation Techniques Provide Data Fusion and Optimal Analysis Frameworks

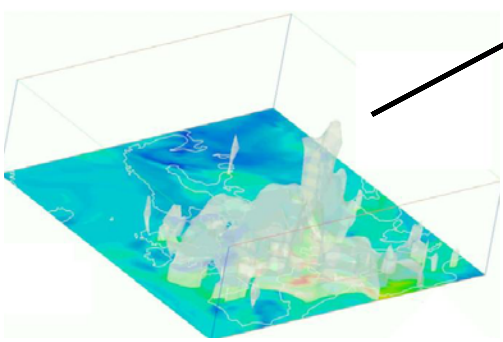
Model ~~vs.~~ + Observations

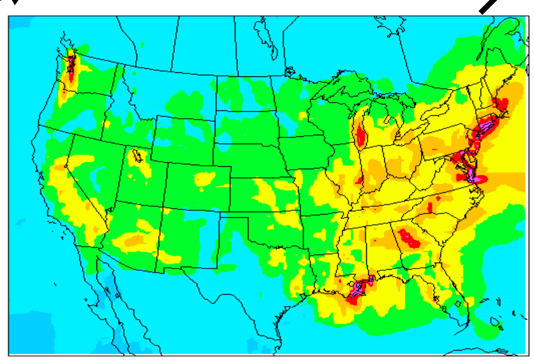


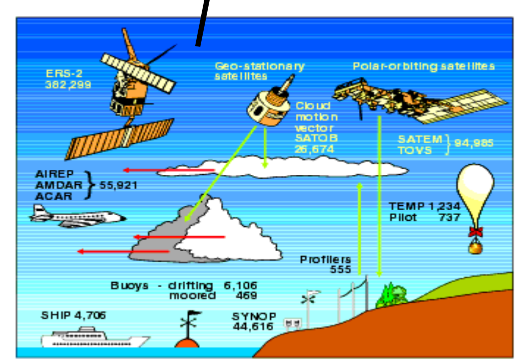
Example 4dVar:

Cost function

$$\min_{\mathbf{y}} \psi(\mathbf{y}) = \left\|\mathbf{y}-\mathbf{y}^{\mathbf{b}}\right\|^2_{\mathbf{B}^{-1}} + \left\|\mathbf{H}\cdot M(\mathbf{y}) - \mathbf{o}\right\|^2_{\mathbf{R}^{-1}}$$







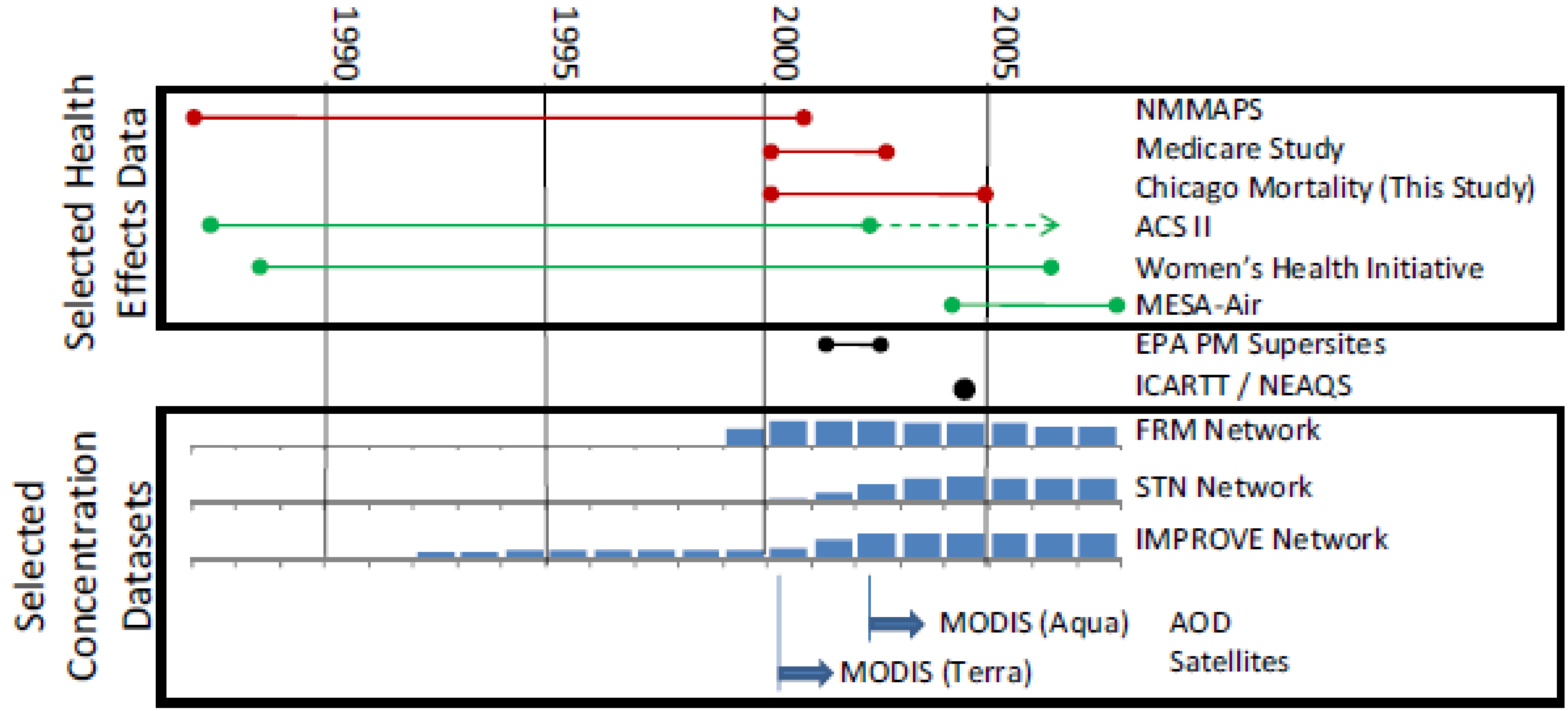
Current knowledge of the state

Model information consistent with physics/chemistry

Observations information consistent with reality

Objective II – Health Studies

Objective 2. Test the utility of the data assimilation exposure estimates by using them in demonstration scale health effects studies for 2001-2004 using ACS II cohort data in selected U.S. cities and geocoded daily mortality time series data from Chicago.


1990
1995
2000
2005
Selected Health Effects Data
NMMAPS
Medicare Study
Chicago Mortality (This Study)
ACS II
Women's Health Initiative
MESA-Air
EPA PM Supersites
ICARTT / NEAQS
Selected Concentration Datasets
FRM Network
STN Network
IMPROVE Network
MODIS (Aqua)
MODIS (Terra)
AOD Satellites

Objective II – Health Studies

Chicago Data Set – secured by Kumar

- Compute daily estimates of total and source-resolved PM2.5 using all the methods from objective 1 for census tracts within the city of Chicago. The coarse U.S. grid will be nested to a 4 km grid over Chicago.
- Time series demonstration study
  - Using GLM with natural cubic spline, examine the daily cause-specific mortality to total and source-resolved PM2.5 with and without DA; Examine daily cause-specific mortality with reference to daily source-resolved PM2.5 at census tract level using a Bayesian hierarchical approach.

ACS II – secured by Krewski with appropriate human subjects oversight by Research Ethics Board of the Ottawa Hospital

- Chronic exposure demonstration using ACS II mortality data
  - Calculate long term average source-specific PM2.5 for Chicago using the range of methods from objective 1.
  - Using spatial analysis techniques developed in previous work by Krewski and colleagues (standard and spatial random effects Cox proportional hazard models), evaluate source-specific relative risks vs. that of total PM.

Synergistic Work of co-I Krewski

- Extended follow-up and spatial analysis of the American Cancer Society Study linking particulate air pollution and mortality (HEI funded)
- Characteristics of PM associated with health effects (HEI funded, with George Thurston)
- Spatiotemporal Analysis of Air Pollution and Mortality in California Based on the American Cancer Society Cohort (Krewski, Michael Jerrett and others)

HEI

RESEARCH REPORT

HEALTH EFFECTS INSTITUTE

Number 140
May 2009

WEB VERSION
Posted
June 3, 2009

Extended Follow-Up and Spatial Analysis of the American Cancer Society Study Linking Particulate Air Pollution and Mortality

Daniel Krewski, Michael Jerrett, Richard T. Burnett, Renjun Ma, Edward Hughes, Yuanli Shi, Michelle C. Turner, C. Arden Pope III, George Thurston, Eugenia E. Calle, and Michael J. Thun

with Bernie Beckerman, Pat DeLuca, Norm Finkelstein, Kaz Ito, D.K. Moore, K. Bruce Newbold, Tim Ramsay, Zev Ross, Hwashin Shin, and Barbara Tempalski

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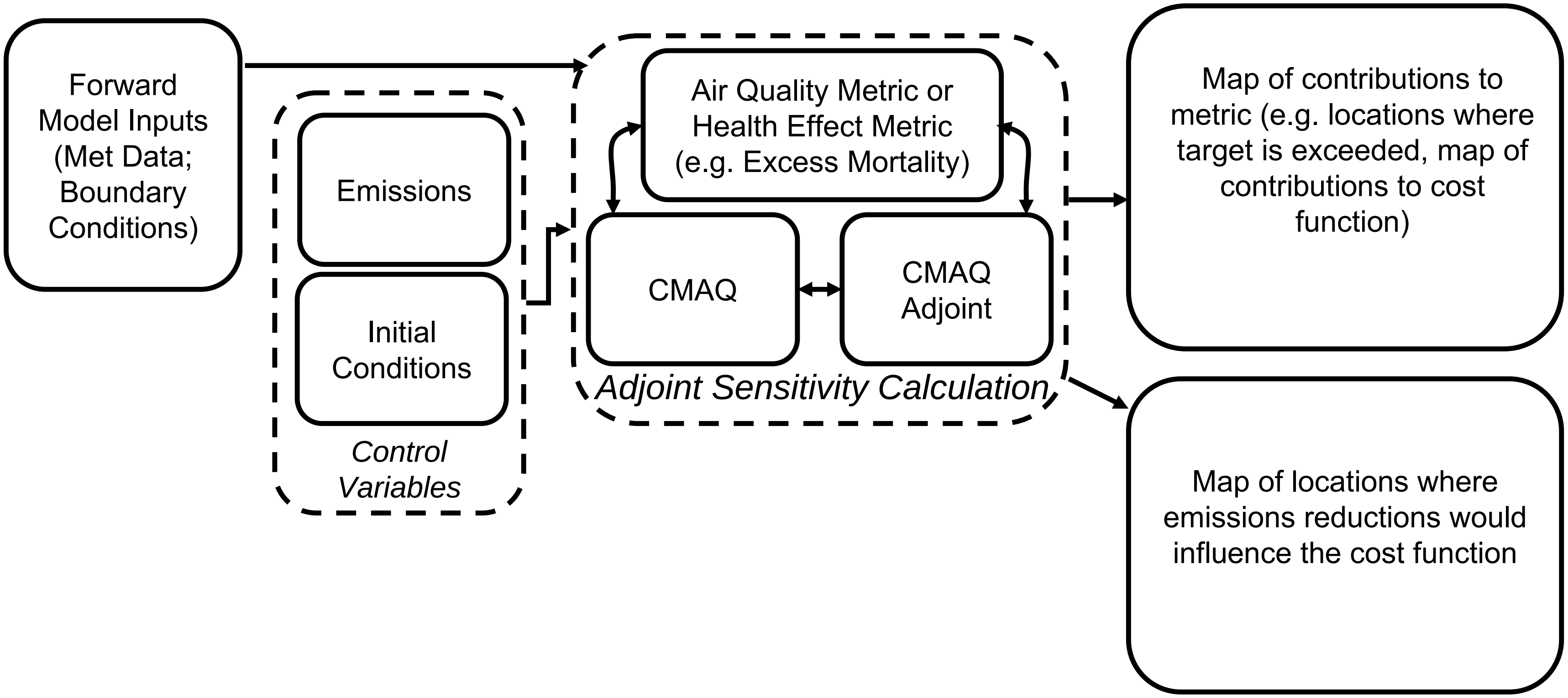
- For Chicago analysis, Kumar and Oleson are developing a Bayesian hierarchical modeling framework to evaluate PM-mortality associations.
- See Oleson and Kumar *A dynamic spatio-temporal autoregressive model for areal data* 2007.

Objective III – Target Oriented Modeling

- Objective 3. Demonstrate the unique potential of target-oriented and adjoint sensitivities relative to the source-resolved PM health effects problem.
  - (i) population weighted PM2.5 exposure in excess of EPA standards;
  - (ii) same as i but with a sensitive population such as eldery patients with comprised respiratory function; and
  - (iii) hypothetical excess mortality from a two source PM mixture (e.g. secondary sulfate and light duty gasoline PM).
- Generate sample surfaces showing sensitivity of these targets to spatial patterns in emissions.



Requires extension of CMAQ-ADJ to include a simplified aerosol adjoint based on the GEOS-CHEM adjoint (Henze, D.K., A. Hakami, and J.H. Seinfeld, *Development of the adjoint of GEOS-Chem.* Atmospheric Chemistry And Physics, 2007. **7**(9): p. 2413-2433)

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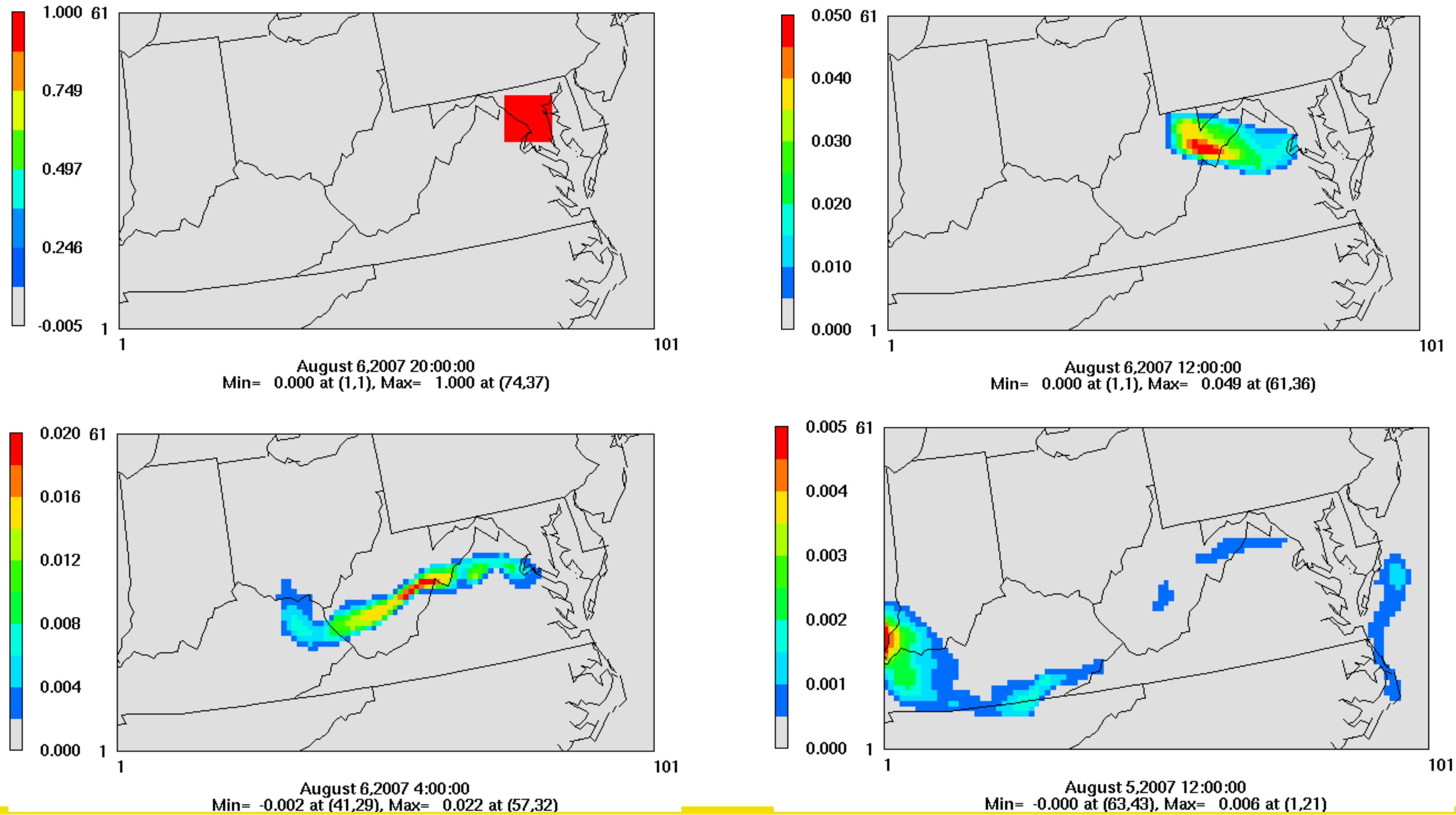
Target Oriented Example



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Thank you

Questions

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